Connecting via Winsock to STN

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LOGINID:ssspta1201txs

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced
NEWS	16	APR 18	New CAS Information Use Policies available online

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:37:53 ON 21 APR 2005

```
=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

FILE 'REGISTRY' ENTERED AT 10:38:01 ON 21 APR 2005
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STRUCTURE FILE UPDATES:   20 APR 2005  HIGHEST RN 848887-73-0
DICTIONARY FILE UPDATES:  20 APR 2005  HIGHEST RN 848887-73-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10706448.str
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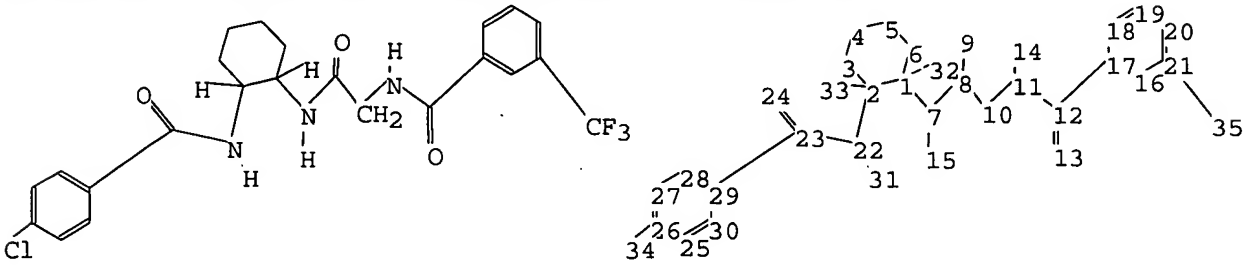


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chain nodes :
7  8  9  10  11  12  13  14  15  22  23  24  31  32  33  34  35
ring nodes :
```

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chain bonds :
1-7  1-32  2-22  2-33  7-8  7-15  8-9  8-10  10-11  11-12  11-14  12-13  12-17
21-35  22-23  22-31  23-24  23-29  26-34
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  16-17  16-21  17-18  18-19  19-20  20-21  25-26
25-30  26-27  27-28  28-29  29-30
exact/norm bonds :
1-7  2-22  7-8  8-9  11-12  12-13  22-23  23-24
exact bonds :
1-2  1-6  1-32  2-3  2-33  3-4  4-5  5-6  7-15  8-10  10-11  11-14  12-17  21-35
22-31  23-29  26-34
normalized bonds :
16-17  16-21  17-18  18-19  19-20  20-21  25-26  25-30  26-27  27-28  28-29  29-30
isolated ring systems :
containing 1 : 16 : 25 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
 11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:Atom  17:Atom  18:Atom
19:Atom  20:Atom  21:Atom  22:CLASS  23:CLASS  24:CLASS  25:Atom  26:Atom  27:Atom
28:Atom  29:Atom  30:Atom  31:CLASS  32:CLASS  33:CLASS  34:CLASS  35:CLASS



L1      STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 10:38:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      7 TO ITERATE

100.0% PROCESSED       7 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            7 TO      298
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 10:38:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    191 TO ITERATE

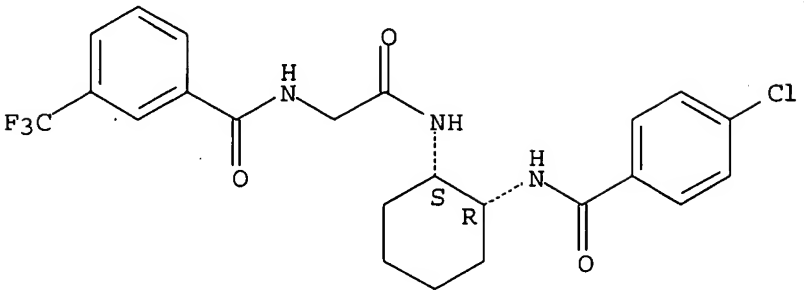
100.0% PROCESSED     191 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

L3            1 SEA SSS FUL L1

=> d scan

L3   1 ANSWERS   REGISTRY  COPYRIGHT 2005 ACS on STN
IN   Benzamide, N-[2-[[(1R,2S)-2-[(4-chlorobenzoyl)amino]cyclohexyl]amino]-2-
     oxoethyl]-3-(trifluoromethyl)-, rel- (9CI)
MF   C23 H23 Cl F3 N3 O3
```

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 10:38:47 ON 21 APR 2005
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 10:37:53 ON 21 APR 2005)

FILE 'REGISTRY' ENTERED AT 10:38:01 ON 21 APR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 1 S L1 FUL

FILE 'CAPLUS' ENTERED AT 10:38:47 ON 21 APR 2005

=> s l3
L4 1 L3

=> d l4 ibib hitstr abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:594806 CAPLUS
DOCUMENT NUMBER: 137:154762
TITLE: Preparation of N-[2-(cycloalkylamino)-2-oxoethyl]benzamides and related compounds as modulators of chemokine receptor activity
INVENTOR(S): Cherney, Robert
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002060859	A2	20020808	WO 2001-US50252		20011220
WO 2002060859	A3	20030327			
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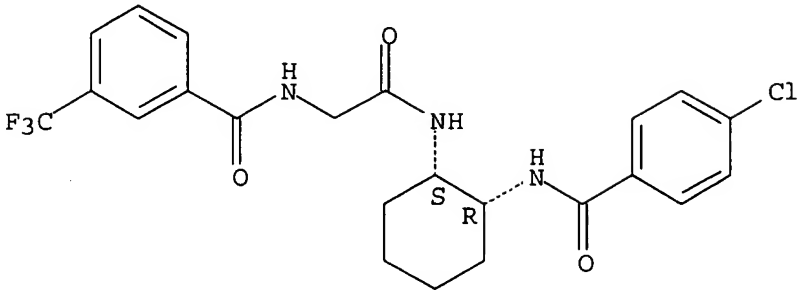
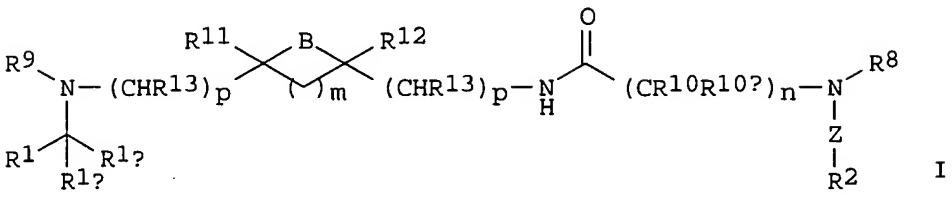
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2432369	AA	20020808	CA 2001-2432369		20011220
US 2003004151	A1	20030102	US 2001-27644		20011220
US 6706712	B2	20040316			
EP 1343751	A2	20030917	EP 2001-997125		20011220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004523534	T2	20040805	JP 2002-561010		20011220
US 2004110736	A1	20040610	US 2003-706448		20031112
PRIORITY APPLN. INFO.:			US 2000-256904P	P	20001220
			US 2001-27644	A3	20011220
			WO 2001-US50252	W	20011220

OTHER SOURCE(S): MARPAT 137:154762
IT **445479-10-7P**, N-[2-[[cis-2-[(4-Chlorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)
RN 445479-10-7 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-chlorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

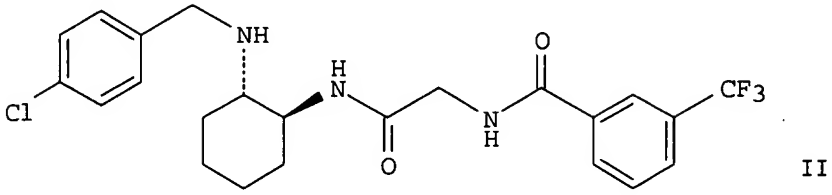
Relative stereochemistry.



GI



I



II

AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepared as modulators of chemokine receptor activity, especially monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addition of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple sclerosis, atherosclerosis and asthma (no data).

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.24	172.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION

CA SUBSCRIBER PRICE -0.73 -0.73

FILE 'REGISTRY' ENTERED AT 10:47:15 ON 21 APR 2005
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STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0
DICTIONARY FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

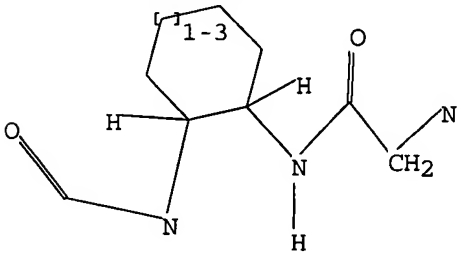
Please note that search-term pricing does apply when conducting SmartSELECT searches.

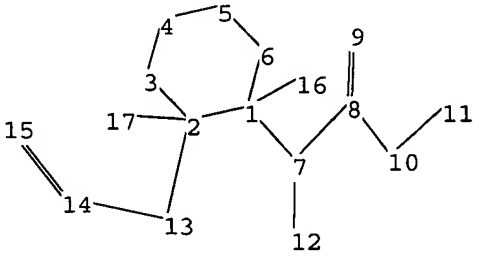
```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\107064481.str





chain nodes :
7 8 9 10 11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 1-16 2-13 2-17 7-8 7-12 8-9 8-10 10-11 13-14 14-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-7 2-13 7-8 8-9 13-14 14-15
exact bonds :

1-2 1-6 1-16 2-3 2-17 3-4 4-5 5-6 7-12 8-10 10-11
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L5 STRUCTURE UPLOADED

=> s l5
SAMPLE SEARCH INITIATED 10:47:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS 9 ANSWERS
SEARCH TIME: 00.00.03

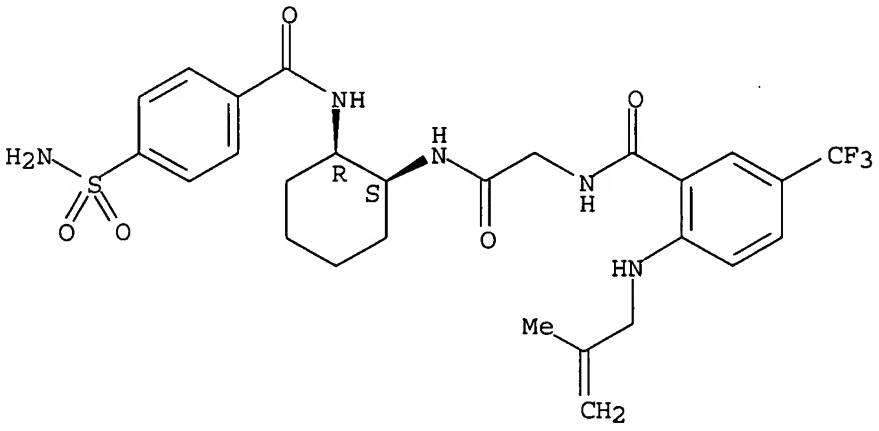
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 833 TO 1807
PROJECTED ANSWERS: 9 TO 360

L6 9 SEA SSS SAM L5

=> d scan

L6 9 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)-, rel-(9CI)
MF C27 H32 F3 N5 O5 S

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.43	173.21

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.73

FILE 'CAPLUS' ENTERED AT 10:47:57 ON 21 APR 2005
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FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

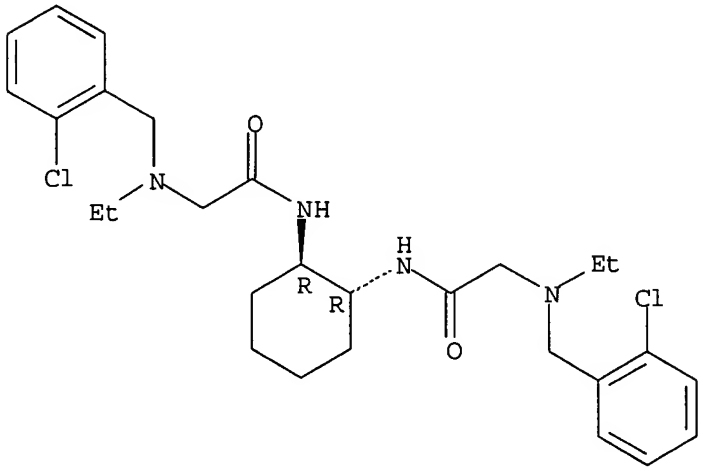
=> s l6
L7 3 L6

=> d l7 ibib hitstr abs 1-3

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:725942 CAPLUS
DOCUMENT NUMBER: 140:209900
TITLE: Design, synthesis and biological evaluation of ambenonium derivatives as AChE inhibitors
AUTHOR(S): Bolognesi, Maria Laura; Cavalli, Andrea; Andrisano, Vincenza; Bartolini, Manuela; Banzi, Rita; Antonello, Alessandra; Rosini, Michela; Melchiorre, Carlo
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Bologna, Bologna, I-40126, Italy
SOURCE: Farmaco (2003), 58(9), 917-928
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **664338-93-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design, synthesis and biol. evaluation of ambenonium derivs. as AChE

inhibitors)
RN 664338-93-6 CAPLUS
CN Acetamide, N,N'-(1R,2R)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Ambenonium, an old AChE inhibitor, is endowed with an outstanding affinity and a peculiar mechanism of action that, taken together, make it a very promising pharmacol. tool for the treatment of Alzheimer's disease (AD). Unfortunately, the bisquaternary structure of ambenonium prevents its passage through the blood brain barrier. In a search of centrally active ambenonium derivs., we planned to synthesize tertiary amines of ambenonium. In addition, to add new insights into the binding mechanism of the inhibitor, we designed constrained analogs of ambenonium by incorporating the diamine functions into cyclic moieties. The biol. evaluation of the new compds. has been assessed in vitro against human AChE and BChE. All tertiary amine derivs. resulted more than 1000-fold less potent than ambenonium and, unlike prototype, did not show any selectivity between the two enzymes. This result, because of recent findings concerning the role of BChE in AD, makes our compds., endowed with a well-balanced profile of AChE/BChE inhibition, valuable candidates for further development. To better clarify the interactions that account for the high affinity of ambenonium, docking simulations and mol. dynamics studies on the AChE-1 complex were also carried out.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:594806 CAPLUS
DOCUMENT NUMBER: 137:154762
TITLE: Preparation of N-[2-(cycloalkylamino)-2-oxoethyl]benzamides and related compounds as modulators of chemokine receptor activity
INVENTOR(S): Cherney, Robert
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002060859	A2	20020808	WO 2001-US50252		20011220
WO 2002060859	A3	20030327			
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2432369	AA	20020808	CA 2001-2432369		20011220
US 2003004151	A1	20030102	US 2001-27644		20011220
US 6706712	B2	20040316			
EP 1343751	A2	20030917	EP 2001-997125		20011220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004523534	T2	20040805	JP 2002-561010		20011220
US 2004110736	A1	20040610	US 2003-706448		20031112
PRIORITY APPLN. INFO.:			US 2000-256904P	P	20001220
			US 2001-27644	A3	20011220
			WO 2001-US50252	W	20011220

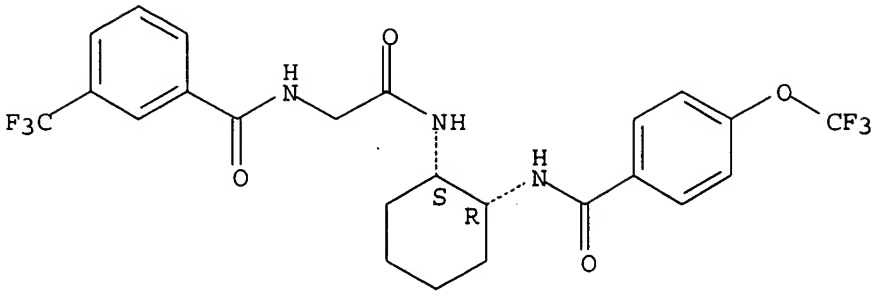
OTHER SOURCE(S): MARPAT 137:154762

IT **445479-21-0P**, N-[2-[[cis-2-[(4-Trifluoromethoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-26-5P**, N-[2-[[cis-2-[(4-Methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-42-5P**, 2-Amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-chlorobenzamide **445479-49-2P**, 4-(Aminosulfonyl)-N-[cis-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]benzamide **445479-57-2P**, 2-(Benzylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-65-2P**, 2-[(2-Methyl-2-propenyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445479-21-0 CAPLUS

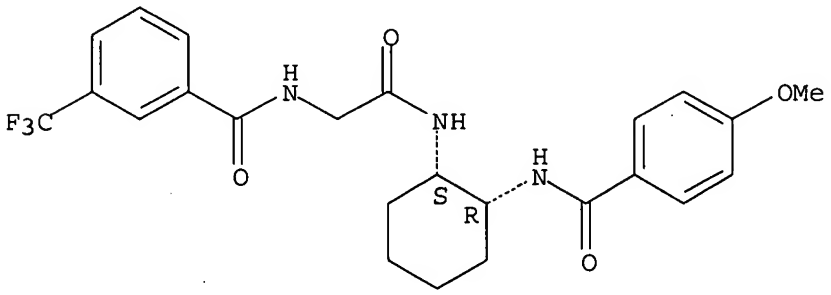
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(trifluoromethoxy)benzoyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



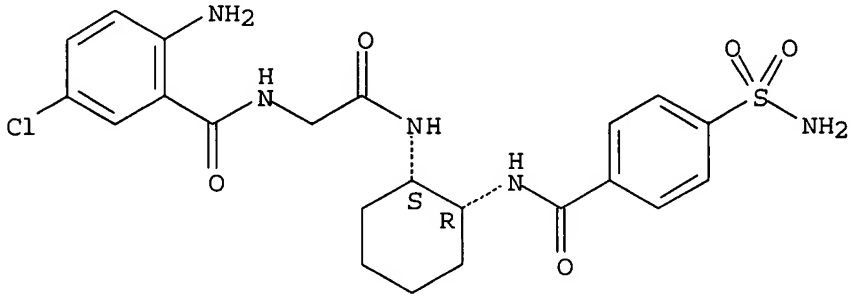
RN 445479-26-5 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



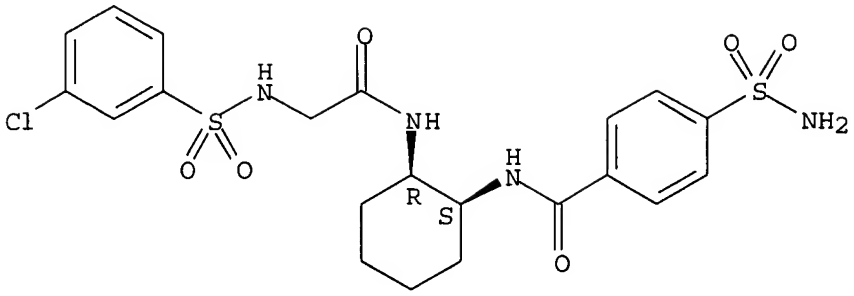
RN 445479-42-5 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-chloro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



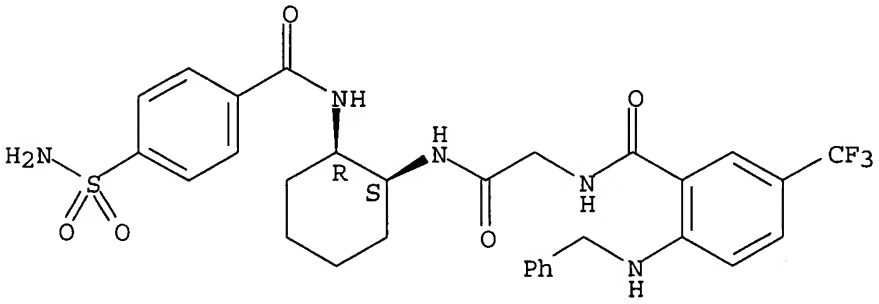
RN 445479-49-2 CAPLUS
CN Benzamide, 4-(aminosulfonyl)-N-[(1R,2S)-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



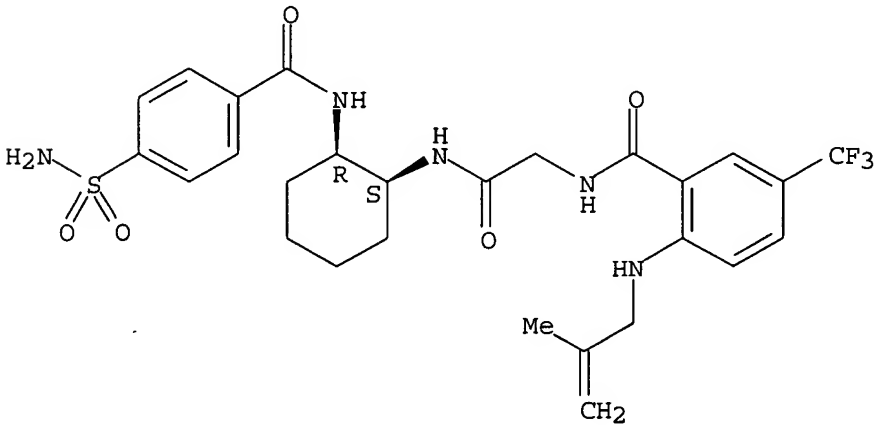
RN 445479-57-2 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(phenylmethyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445479-65-2 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



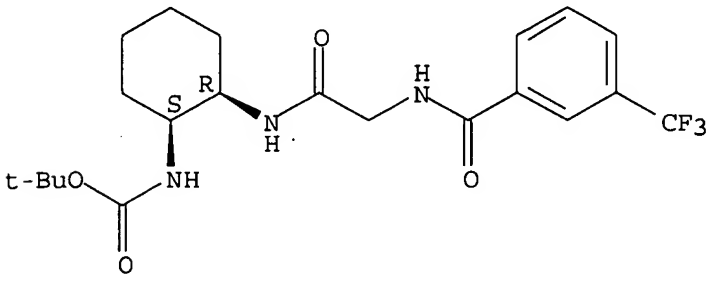
IT **445479-11-8P**, [cis-2-[[[[3-(Trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]carbamic acid 1,1-dimethylethyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445479-11-8 CAPLUS

CN Carbamic acid, [(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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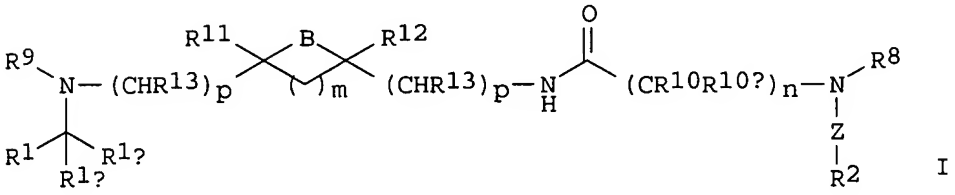

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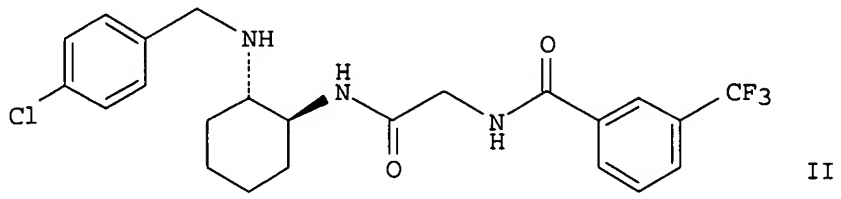


II

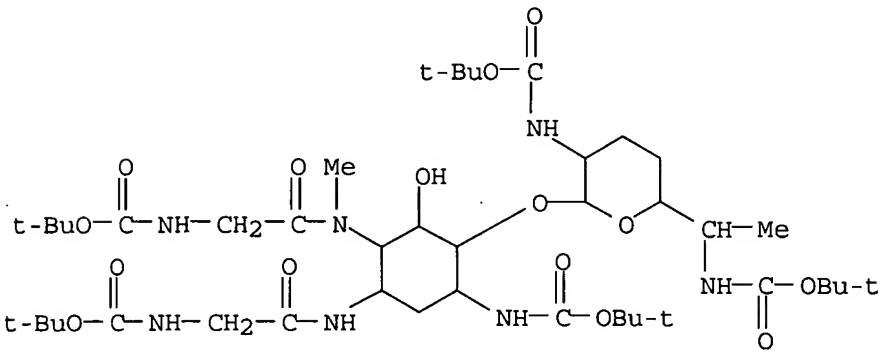
AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepared as modulators of chemokine receptor activity, especially monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addition of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple sclerosis, atherosclerosis and asthma (no data).

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:168775 CAPLUS
DOCUMENT NUMBER: 104:168775
TITLE: Amine glycosides and their use
INVENTOR(S): Loibner, Hans; Streicher, Wolfgang
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 3445646	A1	19851003	DE 1984-3445646		19841214
PRIORITY APPLN. INFO.:			CH 1984-1444	A	19840322

IT **101490-82-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deprotection of)
RN 101490-82-8 CAPLUS
CN L-chiro-Inositol, 1,2,3,6-tetradeoxy-3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]-6-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]methylamino]-4-O-[2,3,4,6,7-pentadeoxy-2,6-bis[[(1,1-dimethylethoxy)carbonyl]amino]-α-D-ribo-heptopyranosyl]- (9CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.
AB Bactericidal (no data) title compds. (I; R1 = H, alkyl; R2 = OH, NH2; R3, R4 = H, OH; R5 = OH, NH2, MeNH; R6 = H, Me; R7 = glycyl) were prepared Thus, 2',3,3'',6'-tetrakis-N-(tert-butoxycarbonyl)gentamicin C2 was oxidized with KMnO4 in aqueous Me2CO to give the 1-deamino-1-nitro derivative which was hydrogenated, N-acylated with a protected glycine derivative, and deprotected to give 6'-epifortimicin derivative II.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	17.97	191.18
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.19	-2.92

FILE 'REGISTRY' ENTERED AT 10:52:12 ON 21 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0
DICTIONARY FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

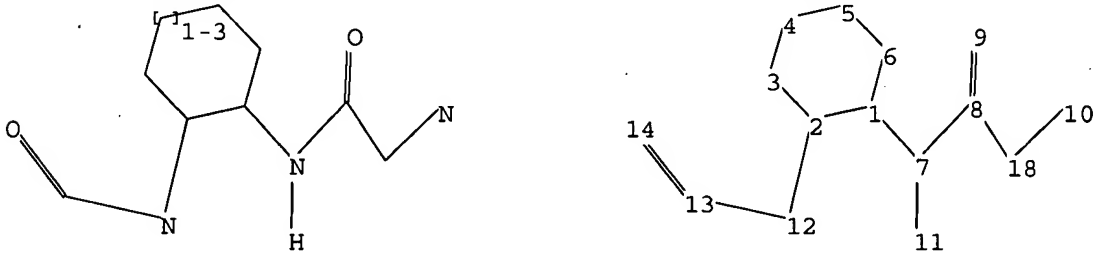
Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\107064482.str



chain nodes :
7 8 9 10 11 12 13 14 18
ring nodes :
1 2 3 4 5 6
chain bonds :
1-7 2-12 7-8 7-11 8-9 8-18 10-18 12-13 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-7 2-12 7-8 8-9 10-18 12-13 13-14
exact bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-11 8-18

isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 18:CLASS

L8 STRUCTURE UPLOADED

=> s l8
SAMPLE SEARCH INITIATED 10:52:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED 66 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

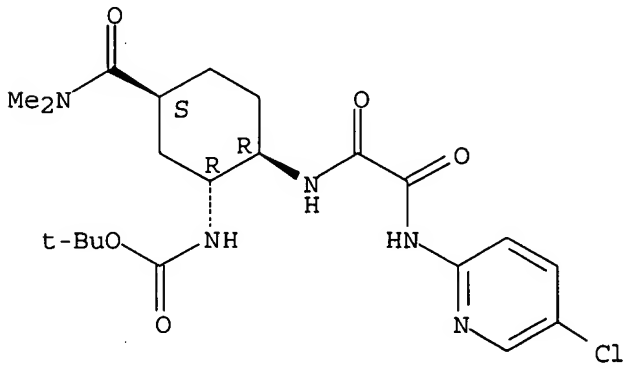
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 833 TO 1807
PROJECTED ANSWERS: 200 TO 800

L9 25 SEA SSS SAM L8

=> d scan

L9 25 ANSWERS REGISTRY COPYRIGHT 2005 ACS on STN
IN Carbamic acid, [(1R,2R,5S)-2-[[[(5-chloro-2-pyridinyl)amino]oxoacetyl]amino]-5-[(dimethylamino)carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI)
MF C21 H30 Cl N5 O5

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	0.43	191.61

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

FILE 'CAPLUS' ENTERED AT 10:52:51 ON 21 APR 2005
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FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	192.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.92

FILE 'REGISTRY' ENTERED AT 10:53:27 ON 21 APR 2005
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STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0
DICTIONARY FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****

```
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> s l8 ful
FULL SEARCH INITIATED 10:53:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1123 TO ITERATE

100.0% PROCESSED    1123 ITERATIONS                          481 ANSWERS
SEARCH TIME: 00.00.01

L10         481 SEA SSS FUL L8

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 161.33     353.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00      -2.92

FILE 'CAPLUS' ENTERED AT 10:53:44 ON 21 APR 2005
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FILE COVERS 1907 - 21 Apr 2005  VOL 142 ISS 17
FILE LAST UPDATED: 20 Apr 2005  (20050420/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> s l10
L11         50 L10
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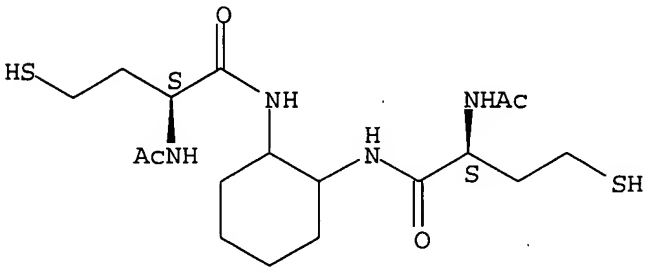
=> d l11 ibib hitstr abs 1-50

L11 ANSWER 2 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:984812 CAPLUS
DOCUMENT NUMBER: 141:415586
TITLE: Preparation of dithiols for hair reinforcement
INVENTOR(S): Philippe, Michel; Andrean, Herve; Barbarat, Philippe
PATENT ASSIGNEE(S): L'oreal, Fr.
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 1477158	A1	20041117	EP 2004-291139		20040504
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
FR 2854797	A1	20041119	FR 2003-5899		20030516
JP 2004339223	A2	20041202	JP 2004-145604		20040514
US 2005019290	A1	20050127	US 2004-846686		20040517
PRIORITY APPLN. INFO.:			FR 2003-5899	A	20030516
			US 2003-477728P	P	20030612

OTHER SOURCE(S): MARPAT 141:415586
IT **791592-24-0P**
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dithiols for hair reinforcement)
RN 791592-24-0 CAPLUS
CN Butanamide, N,N'-1,2-cyclohexanediylbis[2-(acetylamino)-4-mercapto-, (2S,2'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



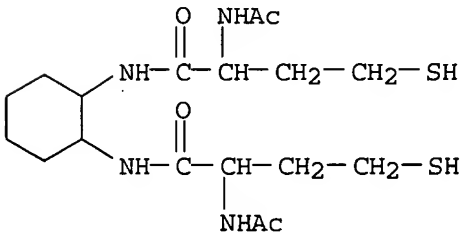
AB Dithiols such as 2-acetylamino-N-[2-(2-acetylamino-4-mercaptobutyrylamino)ethyl]-4-mercaptobutyramide (I) are useful in formulations for strengthening hair. I was prepared by the reaction of ethylenediamine with homocysteine N-acetylthiolactone in CH2Cl2. A formulation contained I 5-15% and water 7-95%.
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:960037 CAPLUS
DOCUMENT NUMBER: 141:400483
TITLE: Amidic dithiols and their use in hair wave preparations for changing the hair form
INVENTOR(S): Philippe, Michel; Andrean, Herve
PATENT ASSIGNEE(S): L'Oreal, Fr.
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 1475076	A1	20041110	EP 2004-291138		20040504
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
FR 2854569	A1	20041112	FR 2003-5497		20030506
JP 2004331663	A2	20041125	JP 2004-136487		20040430
US 2005002886	A1	20050106	US 2004-839233		20040506
PRIORITY APPLN. INFO.:			FR 2003-5497	A	20030506
			US 2003-477726P	P	20030612

OTHER SOURCE(S): MARPAT 141:400483
IT **790227-12-2P**
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(amidic dithiols and their use in hair wave prepns. for changing hair form)
RN 790227-12-2 CAPLUS
CN Butanamide, N,N'-1,2-cyclohexanediylbis[2-(acetylamino)-4-mercapto- (9CI) (CA INDEX NAME)



AB Preparation of amidic dithiols in hair wave prepns. for changing the hair form are disclosed. A solution of ethylenediamine in dichloromethane was reacted with a solution of homocysteine N-aceytlthiolactone in dichloromethane to obtain the amidic dithiol of the composition
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:802720 CAPLUS
DOCUMENT NUMBER: 141:314159
TITLE: Preparation of lactam-containing cyclic diamines and derivatives as factor Xa inhibitors for treating thromboembolic disorders
INVENTOR(S): Qiao, Jennifer X.; Wang, Tammy C.; Wang, Gren Z.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 260 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004082687	A1	20040930	WO 2004-US8088	20040317
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004204454	A1	20041014	US 2004-801469	20040316

PRIORITY APPLN. INFO.:

US 2003-455733P	P	20030318
US 2003-508232P	P	20031002
US 2004-801469	A	20040316

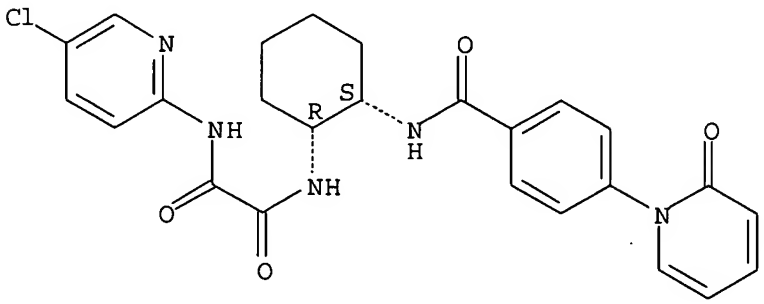
OTHER SOURCE(S): MARPAT 141:314159

IT **766552-69-6P**, N-(5-Chloropyridin-2-yl)-N'-[(1R,2S)-2-[4-(2-oxo-2H-pyridin-1-yl)benzoylamino]cyclohexyl]oxalamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(factor Xa inhibitor; preparation of lactam-containing cyclic diamines and derivs. as factor Xa inhibitors for treating thromboembolic disorders)

RN 766552-69-6 CAPLUS

CN Ethanediamide, N-(5-chloro-2-pyridinyl)-N'-[(1R,2S)-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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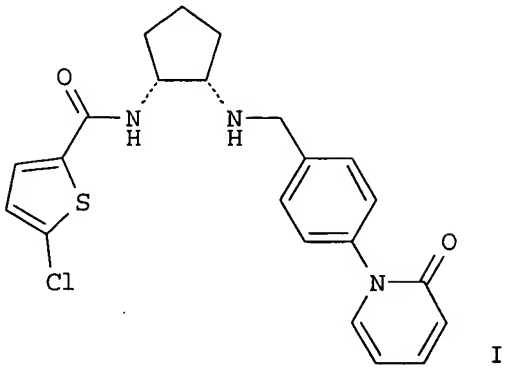
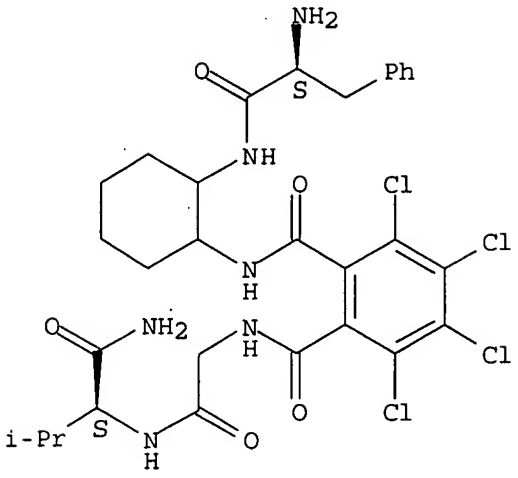


I

AB Title compds. of formula G-G1-M-Z-A-B [wherein M = central ring selected from (un)substituted optionally fused cyclopentane, or cyclohexane, (un)substituted tetrahydropyran, piperidine, piperidin-2-one, pyrrolidine, etc,; G = benzofused ring; G1 = (CH2)1-5 and derivs., (un)substituted CH2:CH2, C(:O), NH, NHCO SO2NH, SO2NHCO, all of the above optionally substituted on one or both ends with alkylene groups, etc., with provisos; Z = NHCO, CONH, Z = (CH2)1-5 and derivs., (un)substituted NHCO, CONH, CO, NHC(:S)NH, S, SO, SO2, SONH, SO2NH, all of the above optionally substituted on one or both ends with alkylene groups, etc.; A = (un)substituted carbo- or heeterocycle; B = lactam or sulfam bound to A ring through an optional linking group attached to the N, pharmaceutically acceptable salts] were prepared as inhibitors of trypsin-like serine proteases, specifically factor Xa, for treating thromboembolic disorders. For example, I was prepared by reductive amination of 4-(2-oxo-2H-pyridin-1-yl)benzaldehyde (preparation given) with (1R,2S)-5-Chlorothiophene-2-carboxylic acid (2-aminocyclopentyl)amide in CH2Cl2 in the presence of NaBH(OAc)3/AcOH. Selected invention compds. displayed Ki ≤ 10 μM in a spectrophotometrical assay using purified human factor Xa.

L11 ANSWER 5 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:751590 CAPLUS
DOCUMENT NUMBER: 141:395799
TITLE: N-tetrachlorophthaloyl (TCP) protection for solid-phase peptide synthesis
AUTHOR(S): Cros, Esther; Planas, Marta; Barany, George; Bardaji, Eduard
CORPORATE SOURCE: Department of Chemistry, University of Girona, Girona, 17071, Spain
SOURCE: European Journal of Organic Chemistry (2004), (17), 3633-3642
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **787635-14-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase peptide synthesis using N-tetrachlorophthaloyl (TCP) protection)
RN 787635-14-7 CAPLUS
CN L-Valinamide, L-phenylalanyl-2-[[(2-aminocyclohexyl)amino]carbonyl]-3,4,5,6-tetrachlorobenzoylglycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The N-tetrachlorophthaloyl-(TCP-)amino protecting group has been evaluated for use in solid-phase peptide synthesis. The TCP group was unaffected by exposure to either piperidine or N,N-diisopropylethylamine (DIEA), which suggests compatibility with both Fmoc and Boc solid-phase synthesis protocols. Quant. TCP removal was achieved by treatment with hydrazine/DMF (3:17) at 35 °C for 30 min or with ethylenediamine/DMF (1:200) at 50 °C for 30 min. Several C-terminal peptide amides were synthesized successfully by following protocols that use hydrazine/DMF (3:17) at 40 °C for 1 h for repetitive deprotection. Treatment of TCP-amines with methylamine or with diamines did not give the corresponding amines (deprotected), but rather the appropriate N,N'-disubstituted tetrachlorophthalamides, which corresponds to a single ring-opening step. This observation was harnessed to prepare linear and macrocyclic peptide-arene hybrids based on the mild reaction of the parent TCP compound with 1,3-diaminopropane/DMF (1:49) at 25 °C for 5 min.

REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:701975 CAPLUS
DOCUMENT NUMBER: 141:225304
TITLE: Preparation of cyclohexyl-substituted lactams as cytokine receptor modulating agents
INVENTOR(S): Cherney, Robert J.; Carter, Percy; Duncia, John V.; Gardner, Daniel S.; Santella, Joseph B.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 385 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004071460	A2	20040826	WO 2004-US4418	20040211

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR,

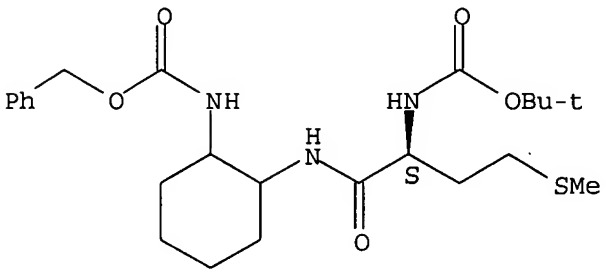
CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES,
ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN,
IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC,
LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX,
MZ, MZ, NA, NI
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU,
MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG

US 2004186140 A1 20040923 US 2004-776828 20040211
PRIORITY APPLN. INFO.: US 2003-446850P P 20030212
OTHER SOURCE(S): MARPAT 141:225304

IT **746670-21-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclohexyl-substituted lactams as modulators for cytokine receptor activity in the treatment of conditions such as inflammation, rheumatoid arthritis, asthma, multiple sclerosis, and atherosclerosis)

RN 746670-21-3 CAPLUS
CN Carbamic acid, [2-[[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-4-(methylthio)-1-oxobutyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

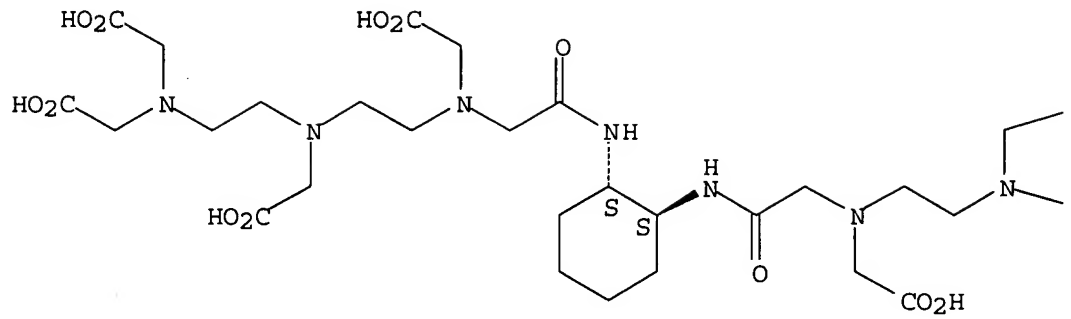
AB Cyclohexyl-substituted lactams I [A = (un)substituted saturated or partially saturated cycloalkyl or heterocycloalkyl group with 3-8 atoms; E = S(:O)pCHR3, CHR3NR3, C(:O)NR3, N(R3)C(:O)NR3, SO2N(R3), N(R3)SO2N(R3); G = (CHR10)n; J = CH2CH2, CH:CH un(substituted) with (R13)s; R1, R2 = (un)substituted aryl or heteroaryl ring; R3 = H, alkyl; R10 = H, (un)substituted alkyl (two R10 groups may together comprise a carbonyl group); R11, R12 (independently) = H, (un)substituted alkyl, aralkyl, heteroaralkyl, ε-hydroxyalkyl, ε-mercaptoalkyl, ε-alkoxyalkyl, etc.; R13 = H, (un)substituted alkyl; X = O, S; Z = bond, (un)substituted aminocarbonyl, aminothiocarbonyl, aminocarbonylamino, aminothiocarbonylamino, aminosulfonyl, aminosulfonylamino, carbonylamino, oxycarbonylamino, aminocarbonyloxy, alkenediyl, methylene, etc.; m = 0-1; n = 0-3; s = 0-1] such as II are prepared as modulators of cytokine activity for the treatment of diseases associated with cytokines and their receptors such as

inflammation, osteo- and rheumatoid arthritis, autoimmune diseases, HIV infection, inflammatory bowel disease, asthma, multiple sclerosis, and atherosclerosis. E.g., 1,4-cyclohexanedione mono(ethylene ketal) is lithiated and acylated with Et cyanoformate, reductively aminated with (S)-α-methylbenzylamine, subjected to reduction with lithium aluminum hydride followed by hydrogenolysis with palladium hydroxide and protection with Cbz anhydride to yield nonracemic III. E.g., III undergoes substitution at the primary carbon with 4-bromophenyl disulfide and tributylphosphine followed by oxidation with mCPBA, Stille methylation of the p-bromophenyl moiety, hydrogenolysis of the Cbz protecting group, acylation with N-Cbz-L-methionine, and S-methylation and cyclization with Me iodide and cesium carbonate to yield IV. E.g., IV undergoes acid-catalyzed deketalization, titanium-mediated Meerwein-Pondorff-Verley reduction with isopropylamine (giving a mixture of both epimers at the amine center), N-methylation with formaldehyde and sodium triacetoxyborohydride, hydrogenolysis of the Cbz protecting group on the aminopyrrolidinone, and acylation with 3-trifluoromethylbenzoic acid and HATU to yield II. The compds. are modulators of chemokine receptor activity (no data). In addition, methods of halolactamization and dehalogenation and reagents appropriate for such transformations are claimed.

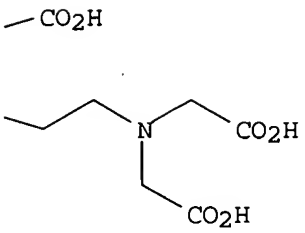
L11 ANSWER 8 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:181386 CAPLUS
DOCUMENT NUMBER: 140:385092
TITLE: Physicochemical characterization of the dimeric lanthanide complexes [en{Ln(DO3A)(H2O)}2] and [pi{Ln(DTTA)(H2O)}2]2-: A variable-temperature 17O NMR study
AUTHOR(S): Lee, Tzu-Ming; Cheng, Tsan-Hwang; Ou, Ming-Hung; Chang, C. Allen; Liu, Gin-Chung; Wang, Yun-Ming
CORPORATE SOURCE: School of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung, 807, Taiwan
SOURCE: Magnetic Resonance in Chemistry (2004), 42(3), 329-336
CODEN: MRCHEG; ISSN: 0749-1581
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **683208-65-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and complexation with lanthanides)
RN 683208-65-3 CAPLUS
CN Glycine, N,N'-[(1R,2R)-1,2-cyclohexanediylbis[imino(2-oxo-2,1-ethanediyl)]]bis[N-[2-[[2-[bis(carboxymethyl)amino]ethyl](carboxymethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



AB The Gd(III) complexes of the two dimeric ligands [en(DO3A)2] {N,N'-bis[1,4,7-tris(carboxymethyl)-1,4,7,10-tetraazacyclododecan-10-ylcarbonylmethyl]-N,N'-ethylenediamine} and [pi(DTTA)2]8-[bis(diethylenetriaminepentaacetic acid) diamide derivative with trans-1,2-cyclohexanediamine] were synthesized and characterized. The 17O NMR chemical shift of H2O induced by [en{Dy(DO3A)}2] and [pi{Dy(DTTA)}2]2- at pH 6.80 proved the presence of 2.1 and 2.2 inner-sphere H2O mols., resp. H2O proton spin-lattice relaxation rates for [en{Gd(DO3A)(H2O)}2] and [pi{Gd(DTTA)(H2O)}2]2- at 37.0 ± 0.1° and 20 MHz are 3.60 ± 0.05 and 5.25 ± 0.05 mM-1 s-1 per Gd, resp. The EPR transverse electronic relaxation rate and 17O NMR transverse relaxation time for the exchange lifetime of the coordinated H2O mol. and the 2H NMR longitudinal relaxation rate of the deuterated diamagnetic La complex for the rotational correlation time were thoroughly studied, and the results were compared with those reported previously for other lanthanide(III) complexes. The exchange lifetimes for [en{Gd(DO3A)(H2O)}2] (769 ± 10 ns) and [pi{Gd(DTTA)(H2O)}2]2- (910 ± 10 ns) are significantly higher than those of [Gd(DOTA)(H2O)]- (243 ns) and [Gd(DTPA)(H2O)]2- (303 ns) complexes. The rotational correlation times for [en{Gd(DO3A)(H2O)}2] (150 ± 11 ps) and [pi{Gd(DTTA)(H2O)}2]2- (130 ± 12 ps) are slightly greater than those of [Gd(DOTA)(H2O)]- (77 ps) and [Gd(DTPA)(H2O)]2- (58 ps) complexes. The marked increase in relaxivity (r1) of [en{Gd(DO3A)(H2O)}2] and [pi{Gd(DTTA)(H2O)}2]2- result mainly from their longer rotational correlation time and higher mol. weight

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

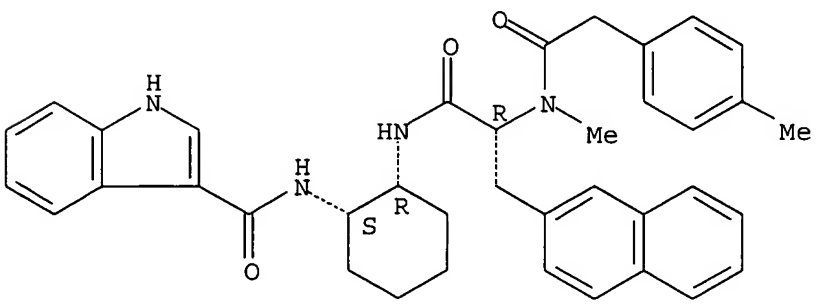
L11 ANSWER 9 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:41273 CAPLUS

DOCUMENT NUMBER: 140:99643
TITLE: Pharmaceutical compositions comprising novel anticholinergic agents and NK1-receptor antagonists for the treatment of respiratory tract diseases
INVENTOR(S): Pairet, Michel; Meade, Christopher John Montague; Pieper, Michael P.
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004004724	A1	20040115	WO 2003-EP6667	20030625
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10230750	A1	20040122	DE 2002-10230750	20020709
EP 1521580	A1	20050413	EP 2003-762508	20030625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004048886	A1	20040311	US 2003-614362	20030707
PRIORITY APPLN. INFO.:			DE 2002-10230750 A	20020709
			US 2002-407758P P	20020903
			WO 2003-EP6667 W	20030625

OTHER SOURCE(S): MARPAT 140:99643
IT **214487-46-4**, MEN-11467
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. comprising anticholinergic agents and NK1-receptor antagonists for treatment of respiratory tract diseases)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The invention relates to novel pharmaceutical compns. comprising novel anticholinergic agents and NK1-receptor antagonists, method for production and use thereof in the treatment of respiratory diseases. Thus an inhalation capsule contained (microgram/capsule): 2,2-Diphenylpropionic acid scopine ester methobromide 200; N-[2-(3,5-Bis-trifluoromethylphenyl)-ethyl]-2-{4-[(3-hydroxypropyl)methylamino]piperidin-1-yl}-N-methyl-2-phenylacetamide 150; lactose 12150.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

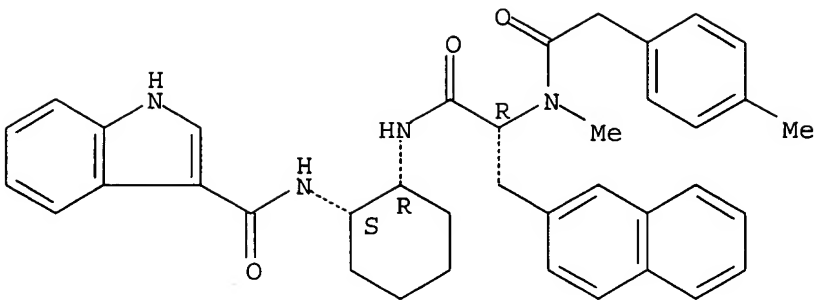
L11 ANSWER 10 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:971894 CAPLUS
DOCUMENT NUMBER: 140:13077
TITLE: Antagonizing NK1 receptors inhibits consumption of substances of abuse
INVENTOR(S): Olive, Michael Foster; Whistler, Jennifer
PATENT ASSIGNEE(S): The Regents of the University of California, USA
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003101459	A1	20031211	WO 2003-US17181	20030529

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-384561P P 20020529
IT **214487-46-4**, MEN 11467
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antagonizing NK1 receptors inhibits consumption of substances of abuse)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB This invention pertains to the surprising discovery that administration of one or more NK1 receptor antagonists to a mammal can inhibit self-administration of a substance of abuse (e.g. alc.). In one embodiment, this invention provides a method of inhibiting or reducing self-administration of a substance of abuse by a mammal. The method involves administering to the mammal an NK1 receptor antagonist in a concentration sufficient to reduce self-administration of a substance of abuse and/or craving for a substance of abuse (e.g. ethanol).

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:737529 CAPLUS
DOCUMENT NUMBER: 139:276714
TITLE: Preparation of arylthiomethyl carbamoylcyclohexanes and related compounds as modulators of chemokine receptor activity
INVENTOR(S): Cherney, Robert J.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 293 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003075853	A2	20030918	WO 2003-US7145	20030307
WO 2003075853	A3	20040401		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003216434	A1	20031120	US 2003-383391	20030307
EP 1483241	A2	20041208	EP 2003-714009	20030307
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: US 2002-362604P P 20020308
WO 2003-US7145 W 20030307

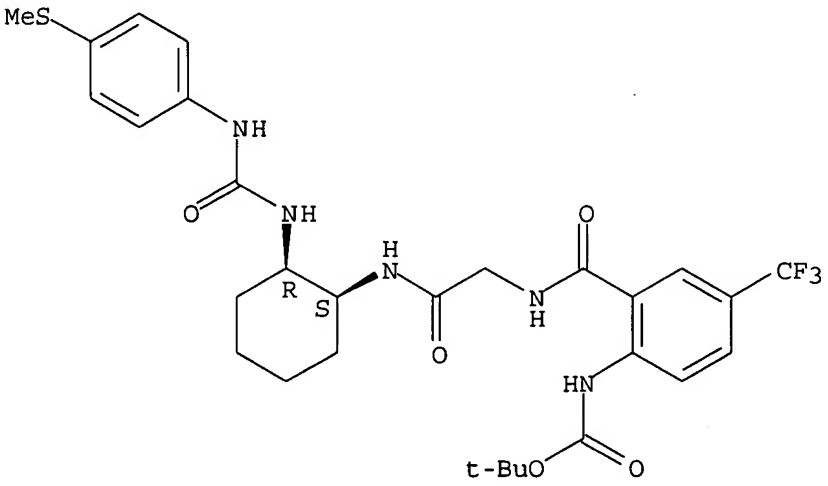
OTHER SOURCE(S): MARPAT 139:276714

IT **604765-26-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylthiomethyl carbamoylcyclohexanes and related compds. as modulators of chemokine receptor activity)

RN 604765-26-6 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[[[4-(methylthio)phenyl]amino]carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB R1E(CHR13)sB(CHR13)sNR14CO(CR10R10a)nN(R8)ZR2 [B = (unsatd.) (substituted) 3-8 membered cycloalkyl, 3-7 membered heterocyclyl; Z = bond, CO, CONH, CSNH, SO2, SO2NH; E = NHCO2, SOpCHR15, COCHR15, etc.; R1, R2 = (substituted) aryl, heteroaryl; R8 = H, alkyl, cycloalkyl; R10, R10a = H, (substituted) alkyl; R13 = Me, (substituted) alkyl; R14, R15 = H, alkyl; n = 1, 2; p = 0-2; s = 0, 1], were prepared as drugs (no data). Thus, (1S*,2R*)(2-phenylsulfanylmethylcyclohexyl)carbamic acid tert-Bu ester (preparation given) in CH2Cl2 at 0° was treated with CF3CO2H and the reaction was warmed to rt to give a residue. This in DMF with diisopropylethylamine and BOC-Gly-OH at 0° was treated with BOP followed by warming to room temperature and stirring overnight. The resulting residue was treated with CF3CO2H in CH2Cl2 at 0° to room temperature to give a residue which in DMF with diisopropylethylamine and 2-(tert-butoxycarbonyl)amino-5-trifluoromethylbenzoic acid at 0° was treated with BOP followed by warming to room temperature and stirring overnight to give tert-Bu 2-[[[2-[[(1S*,2R*)-2-[(phenylthio)methyl]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenylcarbamate.

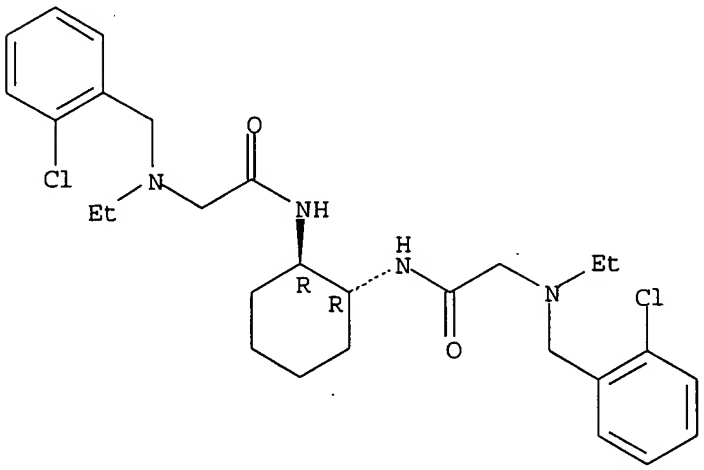
L11 ANSWER 12 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:725942 CAPLUS
DOCUMENT NUMBER: 140:209900
TITLE: Design, synthesis and biological evaluation of ambenonium derivatives as AChE inhibitors
AUTHOR(S): Bolognesi, Maria Laura; Cavalli, Andrea; Andrisano, Vincenza; Bartolini, Manuela; Banzi, Rita; Antonello,

Alessandra; Rosini, Michela; Melchiorre, Carlo
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Bologna, Bologna, I-40126, Italy
SOURCE: Farmaco (2003), 58(9), 917-928
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **664338-93-6P 664338-96-9P 664338-98-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design, synthesis and biol. evaluation of ambenonium derivs. as AChE inhibitors)

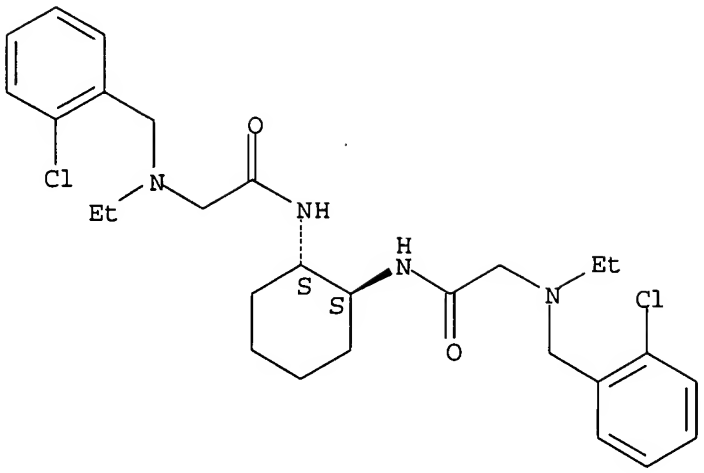
RN 664338-93-6 CAPLUS
CN Acetamide, N,N'-(1R,2R)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



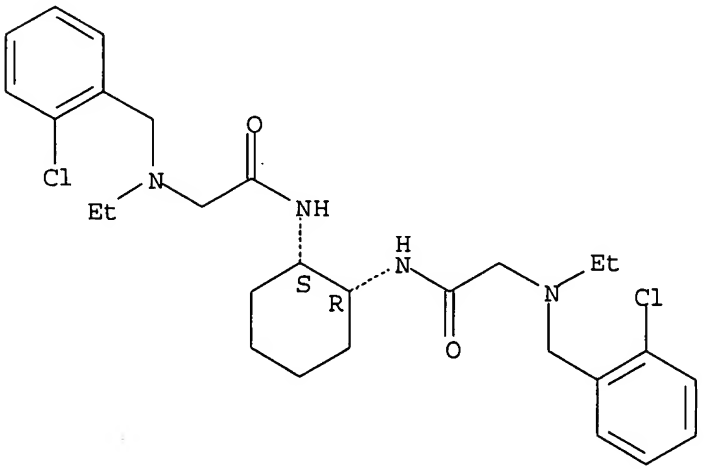
RN 664338-96-9 CAPLUS
CN Acetamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 664338-98-1 CAPLUS
CN Acetamide, N,N'-(1R,2S)-1,2-cyclohexanediylbis[2-[[(2-chlorophenyl)methyl]ethylamino]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



AB Ambenonium, an old AChE inhibitor, is endowed with an outstanding affinity and a peculiar mechanism of action that, taken together, make it a very promising pharmacol. tool for the treatment of Alzheimer's disease (AD). Unfortunately, the bisquaternary structure of ambenonium prevents its passage through the blood brain barrier. In a search of centrally active ambenonium derivs., we planned to synthesize tertiary amines of ambenonium. In addition, to add new insights into the binding mechanism of the inhibitor, we designed constrained analogs of ambenonium by incorporating the diamine functions into cyclic moieties. The biol. evaluation of the new compds. has been assessed in vitro against human AChE and BChE. All tertiary amine derivs. resulted more than 1000-fold less potent than ambenonium and, unlike prototype, did not show any selectivity between the two enzymes. This result, because of recent findings concerning the role of BChE in AD, makes our compds., endowed with a well-balanced profile of AChE/BChE inhibition, valuable candidates for further development. To better clarify the interactions that account

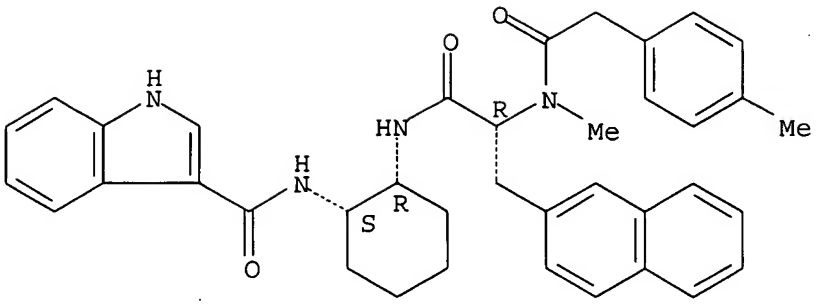
for the high affinity of ambenonium, docking simulations and mol. dynamics studies on the AChE-1 complex were also carried out.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:610660 CAPLUS
DOCUMENT NUMBER: 139:160766
TITLE: A method for correlating the preprotachykinin gene (NKNA) polymorphisms with the efficacy and compatibility of a pharmaceutically active compounds, such as NK-1 receptor antagonists
INVENTOR(S): Foernzler, Dorothee; Hashimoto, Lara; Li, Jia; Luedin, Eric; Sleight, Andrew; Vankan, Pierre
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003064685	A2	20030807	WO 2003-EP630	20030123
WO 2003064685	A3	20031224		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1472377	A2	20041103	EP 2003-734685	20030123
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003007257	A	20041214	BR 2003-7257	20030123
US 2003158187	A1	20030821	US 2003-354693	20030130
PRIORITY APPLN. INFO.:			EP 2002-1937 A	20020131
			WO 2003-EP630 W	20030123

IT **214487-46-4**, MEN 11467
RL: ANT (Analyte); PAC (Pharmacological activity); THU (Therapeutic use); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(NK-1 receptor antagonist; method for correlating preprotachykinin gene (NKNA) polymorphisms with efficacy and compatibility of pharmaceutically active compds., such as NK-1 receptor antagonists)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The present invention relates to a method for correlating single nucleotide polymorphisms in the preprotachykinin (NKNA) gene with the efficacy and compatibility of a pharmaceutically active compound administered to a human being. The invention further relates to a method for determining the efficacy and compatibility of a pharmaceutically active compound administered to a human being which method comprises determining at least one single nucleotide polymorphism in the NKNA gene. Said methods are based on determining specific single nucleotide polymorphisms in the NKNA gene and determining the efficacy and compatibility of a pharmaceutically active compound in the human by reference to polymorphism in NKNA. The invention further relates to isolated nucleic acids comprising within their sequence the polymorphisms as defined herein, to nucleic acid primers and oligonucleotide probes capable of hybridizing to such nucleic acids and to a diagnostic kit comprising one or more of such primers and probes for detecting a polymorphism in the NKNA gene, to a pharmaceutical pack comprising neurokinin-1 (NK-1) receptor antagonists and instructions for administration of the drug to human beings tested for the polymorphisms as well as to a computer readable medium with the stored sequence information for the polymorphisms in the NKNA gene.

L11 ANSWER 18 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:869585 CAPLUS
DOCUMENT NUMBER: 137:346202
TITLE: Pharmaceutical compositions based on anticholinergics and NK1-receptor antagonists for the treatment of respiratory tract diseases
INVENTOR(S): Pairet, Michel; Pieper, Michael P.; Meade, Christopher J. M.
PATENT ASSIGNEE(S): Germany
SOURCE: U.S. Pat. Appl. Publ., 18 pp., Cont.-in-part of U. S. Provisional Ser. NO. 281,653.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002169181	A1	20021114	US 2002-92116	20020306
US 6620438	B2	20030916		
DE 10111058	A1	20020912	DE 2001-10111058	20010308
US 2003212075	A1	20031113	US 2003-419358	20030421
US 6696042	B2	20040224		

US 2004151770	A1	20040805	US 2004-763894		20040123
PRIORITY APPLN. INFO.:			DE 2001-10111058	A	20010308
			US 2001-281653P	P	20010405
			US 2002-92116	A1	20020306
			US 2003-419358	A1	20030421

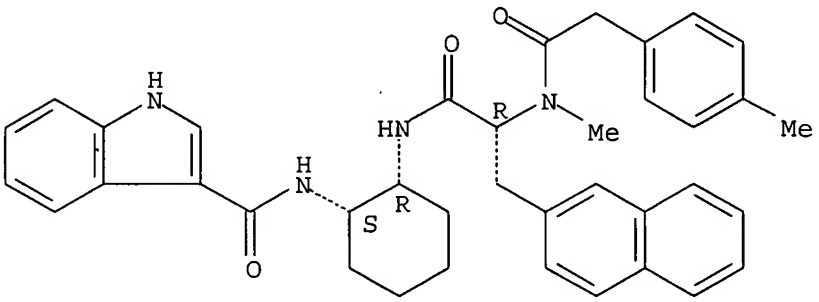
OTHER SOURCE(S): MARPAT 137:346202

IT **214487-46-4**, MEN-11467
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anticholinergics and NK1-receptor antagonists for treatment of respiratory tract diseases)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The invention discloses pharmaceutical compns. based on anticholinergics and NK1-receptor antagonists, processes for preparing them, and their use in the treatment of respiratory tract diseases. Preparation of selected compds. is included.

L11 ANSWER 19 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	2002:832668 CAPLUS
DOCUMENT NUMBER:	137:337901
TITLE:	Preparation and use of amides as NK-1 receptor antagonists against benign prostatic hyperplasia
INVENTOR(S):	Buser, Susanne; Ford, Anthony P. D. W.; Hoffmann, Torsten; Lenz, Barbara; Sleight, Andrew John; Vankan, Pierre
PATENT ASSIGNEE(S):	F. Hoffmann-La Roche A.-G., Switz.
SOURCE:	PCT Int. Appl., 45 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085458	A2	20021031	WO 2002-EP1085	20020202
WO 2002085458	A3	20031030		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,

PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2444395	AA	20021031	CA 2002-2444395	20020202
EP 1385577	A2	20040204	EP 2002-719751	20020202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002009151	A	20040713	BR 2002-9151	20020202
JP 2004529931	T2	20040930	JP 2002-583031	20020202
US 2003004157	A1	20030102	US 2002-71570	20020208
PRIORITY APPLN. INFO.:			EP 2001-109853 A	20010423
			WO 2002-EP1085 W	20020202

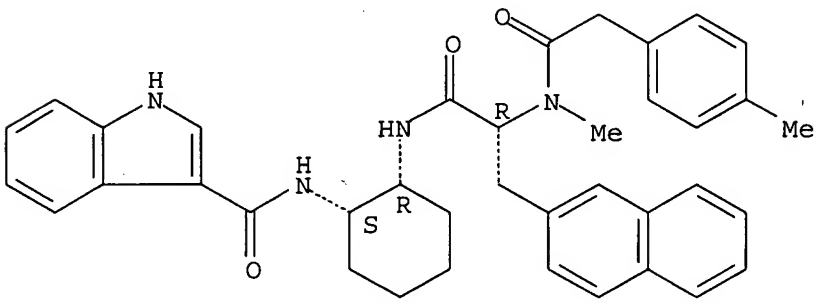
OTHER SOURCE(S): MARPAT 137:337901

IT **214487-46-4**, MEN 11467
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and use of amides as NK-1 receptor antagonists against benign prostatic hyperplasia)

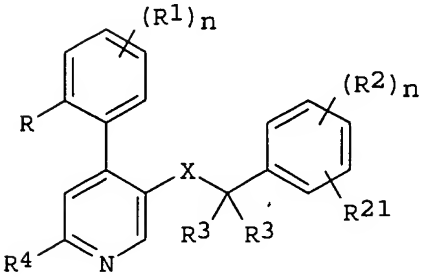
RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



I

AB Use of an NK-1 receptor antagonist for the treatment or prevention of

benign prostatic hyperplasia (BPH) is claimed. The preferred NK-1 receptor antagonists are compds. of the general formula [I; R = H, alkyl, alkoxy, halo, CF3; R1 = H, halo; RR1 = CH:CHCH:CH; R2, R21 = H , halo , CF3, alkyl, alkoxy, cyano; R2R21 = CH:CHCH:CH, optionally substituted by 1-2 alkyl, halo, alkoxy; R3 = H, alkyl; R3R3C = cycloalkyl; R4 = H, N(R5)2, NR5(CH2)nOH, cyclic tertiary amine, etc.; X = CONR5, (CH2)pO, NR5(CH2)p, etc.; R5 = H, cycloalkyl, Ph, PhCH2, alkyl; n = 0-4; p = 1-3]. Preferred compds. are 2-(3,5-bis-trifluoromethyl-phenyl)-N-methyl-N-(6-morpholin-4-yl-4-o-tolyl-pyridin-3-yl)isobutyramide, 3-(3,5-bis-trifluoromethyl-phenyl)-N-methyl-N-[6-(4-methyl-piperazin-1-yl)-4-o-tolyl-pyridin-3-yl]isobutyramide, 2-(3,5-bis-trifluoromethyl-phenyl)-N-[6-(1,1-dioxo-1λ6-thiomorpholin-4-yl)-4-o-tolyl-pyridin-3-yl]-N-methylisobutyramide, and 2-(3,5-bis-trifluoromethylphenyl)-N-[6-(1,1-dioxo-1λ6-thiomorpholin-4-yl)-4-(4-fluoro-2-methyl-phenyl)-pyridin-3-yl]-N-methylisobutyramide. Thus, 2-[3,5-bis(trifluoromethyl)phenyl]-N-methyl-N-(6-thiomorpholin-4-yl-4-o-tolylpyridin-3-yl)isobutyramide (preparation given) oxone were stirred 2 days at room temperature to give 2-(3,5-bis-trifluoromethylphenyl)-N-[6-(1,1-dioxo-1λ6-thiomorpholin-4-yl)-4-o-tolylpyridin-3-yl]-N-methylisobutyramide. 2-(3,5-Bistrifluoromethylphenyl)-N-methyl-N-methyl-N-(6-morpholin-4-yl-4-o-tolylpyridin-3-yl)isobutyramide at 60 mg/kg/day orally in dogs reduced prostate weight by 58% after 39 wk.

L11 ANSWER 20 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:695760 CAPLUS
DOCUMENT NUMBER: 137:237717
TITLE: Inhalant compositions containing anticholinergics and NK1 receptor antagonists
INVENTOR(S): Meade, Christopher John Montague; Pairet, Michel; Pieper, Michael Paul
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002069944	A2	20020912	WO 2002-EP1987	20020226
WO 2002069944	A3	20031002		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10111058	A1	20020912	DE 2001-10111058	20010308
CA 2439915	AA	20020912	CA 2002-2439915	20020226
EP 1370293	A2	20031217	EP 2002-719915	20020226
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004519484	T2	20040702	JP 2002-569121	20020226
PRIORITY APPLN. INFO.:			DE 2001-10111058 A	20010308

WO 2002-EP1987 W 20020226

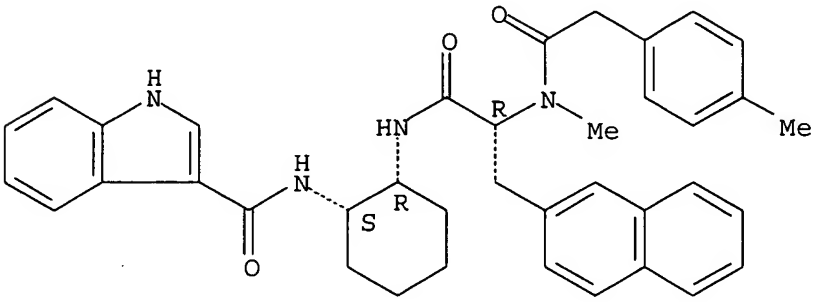
OTHER SOURCE(S): MARPAT 137:237717

IT **214487-46-4**, MEN-11467
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhalant compns. containing anticholinergics and NK1 receptor antagonists)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The invention relates to drug compns. based on anticholinergics and on NK1 receptor antagonists, to methods for their production, and to their use as inhalants for the treatment of respiratory tract diseases. Synthesis of NK1 receptor antagonists from the group of bis-trifluoromethyl-phenyl-piperidine derivs. are described. The products are used in suspension aerosols. Thus a composition contained (weight/weight%): tiotropium bromide 0.015;
NK1 receptor antagonist 0.066; soy lecithin 0.2; TG11: TG12 = 2:3 to 100.

L11 ANSWER 21 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:594806 CAPLUS
DOCUMENT NUMBER: 137:154762
TITLE: Preparation of N-[2-(cycloalkylamino)-2-oxoethyl]benzamides and related compounds as modulators of chemokine receptor activity
INVENTOR(S): Cherney, Robert
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002060859	A2	20020808	WO 2001-US50252	20011220
WO 2002060859	A3	20030327		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2432369	AA	20020808	CA 2001-2432369	20011220
US 2003004151	A1	20030102	US 2001-27644	20011220
US 6706712	B2	20040316		
EP 1343751	A2	20030917	EP 2001-997125	20011220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004523534	T2	20040805	JP 2002-561010	20011220
US 2004110736	A1	20040610	US 2003-706448	20031112
PRIORITY APPLN. INFO.:			US 2000-256904P	P 20001220
			US 2001-27644	A3 20011220
			WO 2001-US50252	W 20011220

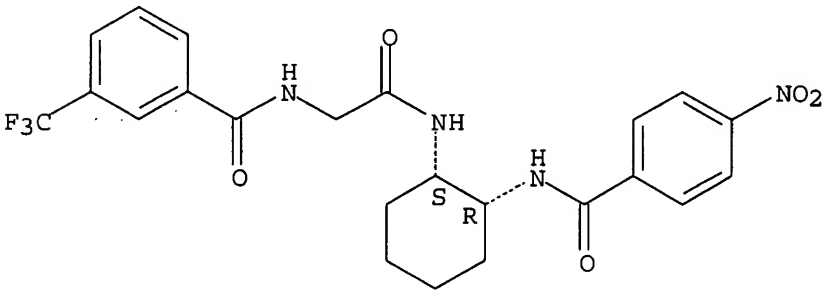
OTHER SOURCE(S): MARPAT 137:154762

IT **445479-24-3P**, N-[2-[[cis-2-[(4-Nitrobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-47-0P** **445479-62-9P** **445480-07-9P**, 2-[(Propyl)amino]-N-[2-[[cis-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-47-7P** **445480-49-9P**, [4-(4-Methylthiobenzoylamino)-3-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid benzyl ester **445480-52-4P** **445480-54-6P**, 1-(4-Methylthiobenzoylamino)-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]-6-aminocyclohexane
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445479-24-3 CAPLUS

CN Benzamide, N-[2-[[(1R,2S)-2-[(4-nitrobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



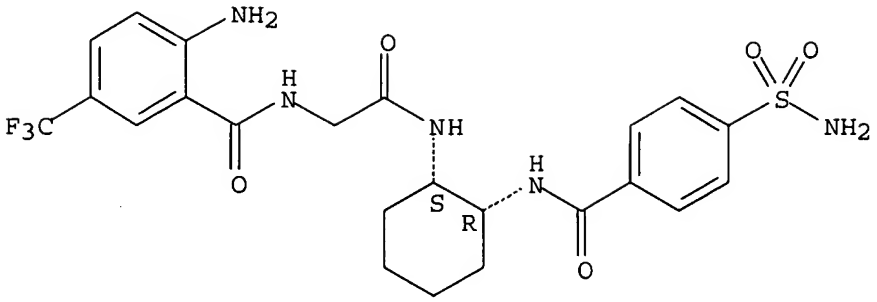
RN 445479-47-0 CAPLUS

CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

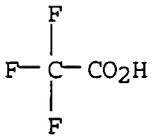
CRN 445479-46-9
CMF C23 H26 F3 N5 O5 S

Relative stereochemistry.



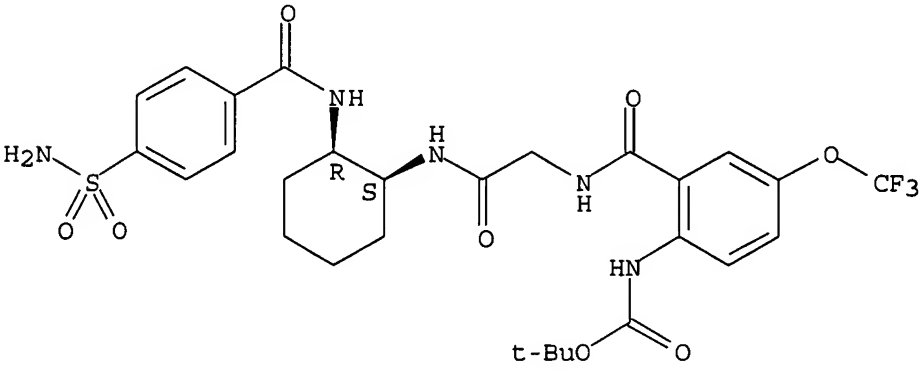
CM 2

CRN 76-05-1
CMF C2 H F3 O2



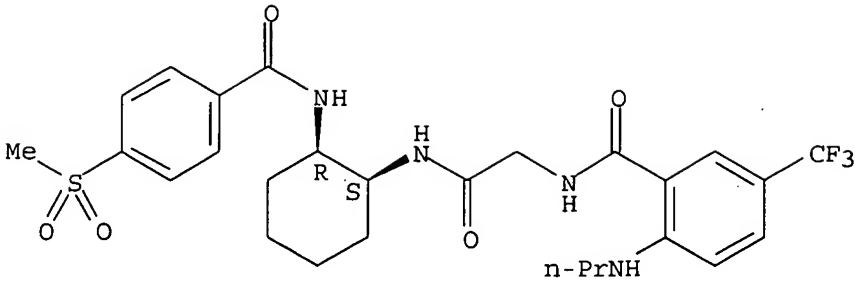
RN 445479-62-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethoxy)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

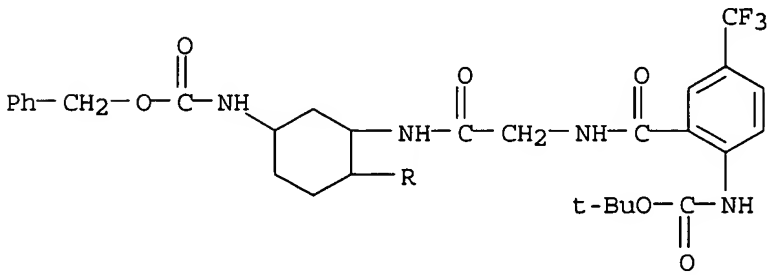


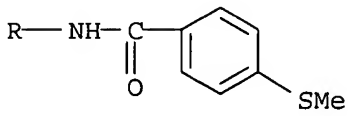
RN 445480-07-9 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]a mino]-2-oxoethyl]-2-(propylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

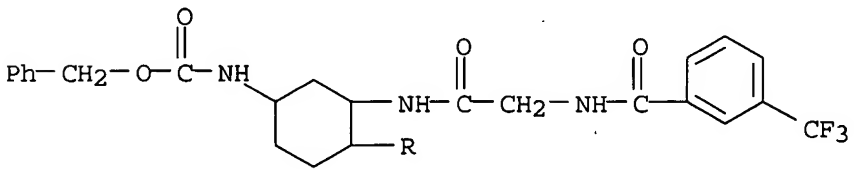


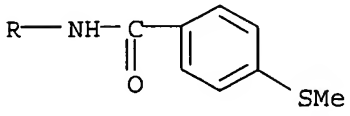
RN 445480-47-7 CAPLUS
CN Carbamic acid, [3-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-4-[[4-(methylthio)benzoyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



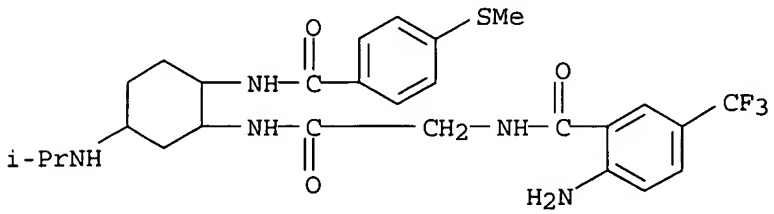


RN 445480-49-9 CAPLUS
CN Carbamic acid, [4-[[4-(methylthio)benzoyl]amino]-3-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

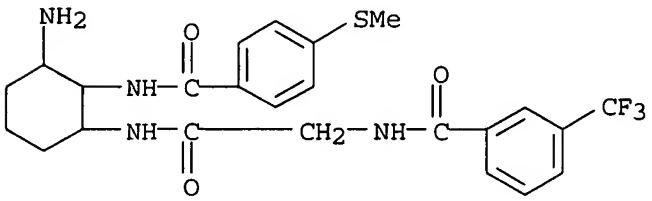




RN 445480-52-4 CAPLUS
CN Benzamide, 2-amino-N-[2-[[5-[(1-methylethyl)amino]-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 445480-54-6 CAPLUS
CN Benzamide, N-[2-[[3-amino-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **445479-10-7P**, N-[2-[[cis-2-[(4-Chlorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-12-9P**, N-[2-[[cis-2-[(4-Methylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-13-0P**, N-[2-[[cis-2-[(4-Fluorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-14-1P**, N-[2-[[cis-2-(Benzoylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-15-2P**, N-[2-[[cis-2-[(4-Bromobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-16-3P**, N-[2-[[cis-2-[(4-Phenoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-17-4P**, N-[2-[[cis-2-[(4-Trifluoromethylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-18-5P 445479-19-6P**, N-[2-[[cis-2-[(4-Iodobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-20-9P**, N-[2-[[cis-2-[(4-Cyanobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-21-0P**, N-[2-[[cis-2-[(4-Trifluoromethoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-22-1P**, N-[2-[[cis-2-[(4-Formylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-23-2P**, N-[2-[[cis-2-[(4-Carbomethoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-25-4P**, N-[2-[[cis-2-[(4-Aminobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-26-5P**, N-[2-[[cis-2-[(4-Methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-27-6P**, N-[2-[[cis-2-[(4-Methylthiobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-28-7P**, N-[2-[[cis-2-[(4-Methylsulfonylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-

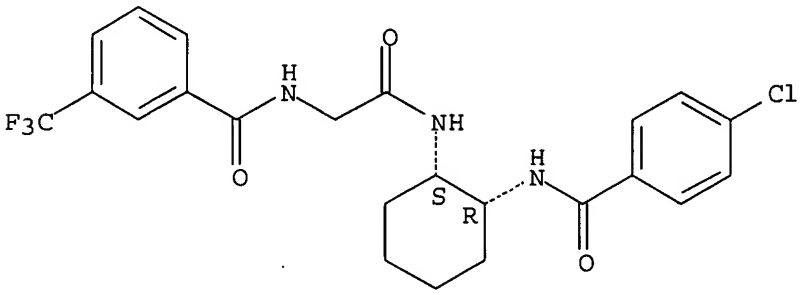
(trifluoromethyl)benzamide **445479-29-8P**, N-[2-[[cis-2-[(4-Aminosulfonylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-30-1P**, N-[2-[[cis-2-[(4-Isopropylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-31-2P**, N-[2-[[cis-2-[(4-Phenylthiobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-32-3P**, N-[2-[[cis-2-[[4-(N,N-Diethylsulfamoyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-33-4P**, N-[2-[[cis-2-[(4-Trifluoromethylthiobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)benzamide **445479-39-0P**, 2-Amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodobenzamide **445479-42-5P**, 2-Amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-chlorobenzamide **445479-43-6P**, N-[2-[[cis-2-[[4-(Aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-chlorobenzamide **445479-44-7P**, N-[2-[[cis-2-[[4-(Aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-trifluoromethoxybenzamide **445479-45-8P 445479-48-1P**, 4-(Aminosulfonyl)-N-[cis-2-[[[[2-(trifluoromethyl)anilino]carbonyl]amino]acetyl]amino]cyclohexyl]benzamide **445479-49-2P**, 4-(Aminosulfonyl)-N-[cis-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]benzamide **445479-50-5P 445479-52-7P 445479-54-9P 445479-56-1P 445479-57-2P**, 2-(Benzylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-58-3P**, 2-(Ethylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-59-4P**, 2-(Methylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-61-8P**, 2-Amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-bromo benzamide **445479-63-0P**, 2-Amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethoxy benzamide **445479-64-1P**, 2-(Allylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-65-2P**, 2-[(2-Methyl-2-propenyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-67-4P 445479-69-6P**, 2-(Butyl)amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-70-9P**, 2-(Propyl)amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-72-1P 445479-74-3P**, 2-[(Aminocarbonyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-76-5P**, 2-(Acetylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-77-6P**, 2-(Methylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodobenzamide **445479-78-7P**, 2-(Ethylamino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodobenzamide **445479-80-1P 445479-82-3P**, 2-Amino-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-nitrobenzamide **445479-83-4P 445479-85-6P 445479-87-8P**, 2-(Amino)-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3,5-dinitrobenzamide **445479-88-9P**, 2-[(Isopropylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-89-0P**,

2-[(Cyclohexylcarbonyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-90-3P**, 2-[(Cyclopentylacetyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-91-4P**, 2-[(Cyclohexylcarbonyl)amino]-N-[2-[[cis-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-trifluoromethylbenzamide **445479-96-9P 445479-97-0P**, 2-[(Isopropylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445479-98-1P**, 2-[(Isopropylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445479-99-2P**, 2-[(Methylsulfonyl)amino]-N-[2-[[cis-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-01-3P 445480-04-6P 445480-05-7P**, 2-[(2-Methyl-2-propenyl)amino]-N-[2-[[cis-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-06-8P**, 2-[(2-Methyl-2-propenyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-08-0P**, 2-[(Propyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-09-1P**, 2-[(2-Methylpropyl)amino]-N-[2-[[cis-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-10-4P 445480-11-5P**, 2-[(2-Methylpropyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-12-6P**, 2-[(Butyl)amino]-N-[2-[[cis-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-13-7P**, 2-[(Butyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-14-8P**, 2-[(Ethylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-16-0P**, 2-[(Allylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-18-2P**, 2-[(Isobutylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-21-7P**, 2-[(Cyclopentylaminocarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-23-9P**, 2-[(tert-Butoxycarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-24-0P**, 2-[(Isopropoxycarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-26-2P**, 2-[(Ethoxycarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-28-4P**, 2-[(Pyrrolidinylcarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-29-5P**, 2-[(Morpholinylcarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-31-9P**, 2-[(Azetidinylcarbonyl)amino]-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide

445480-48-8P 445480-53-5P, 1-(4-Methylthiobenzoylamino)-2-[[2-(2-amino-5-trifluoromethylbenzoylamino)acetyl]amino]-4-(3-methylureido)cyclohexane **445480-57-9P 445480-67-1P**, 4-(4-Methylthiobenzoylamino)-3-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]-4-(2-propylamino)cyclohexane **445480-68-2P**, 1-(4-Methylthiobenzoylamino)-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]-5-aminocyclohexane **445481-22-1P 445481-23-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(chemokine receptor modulator; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

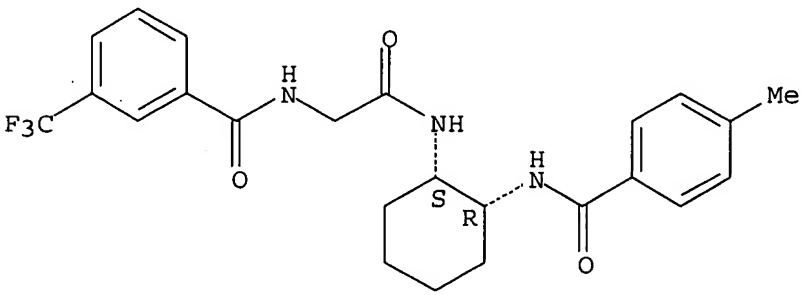
RN 445479-10-7 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-chlorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



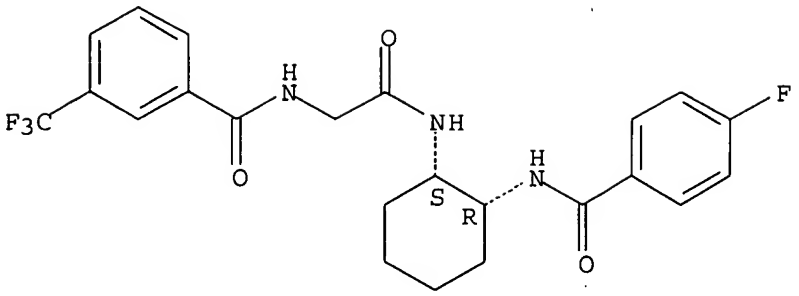
RN 445479-12-9 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-methylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



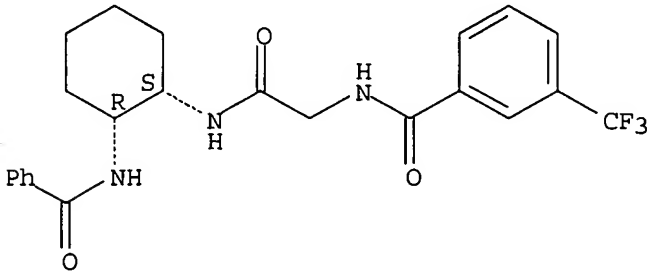
RN 445479-13-0 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-fluorobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



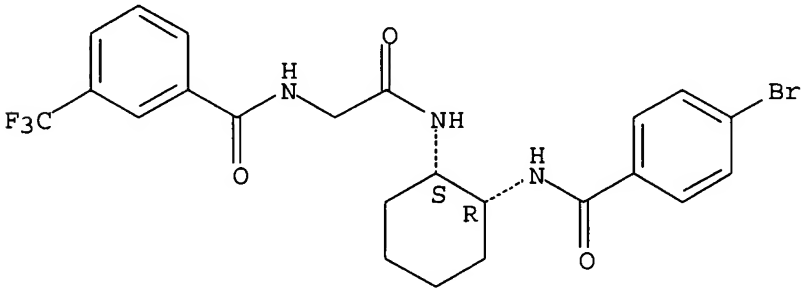
RN 445479-14-1 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-(benzoylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



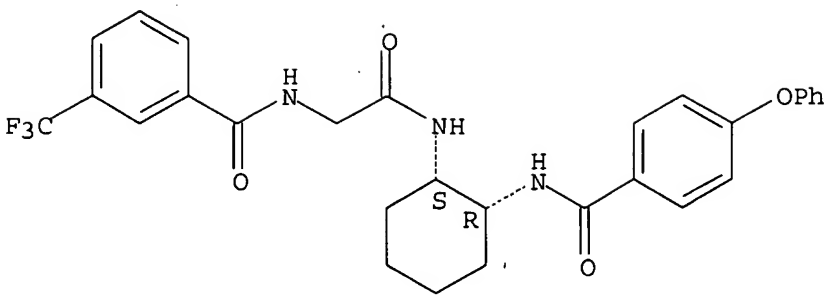
RN 445479-15-2 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-bromobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



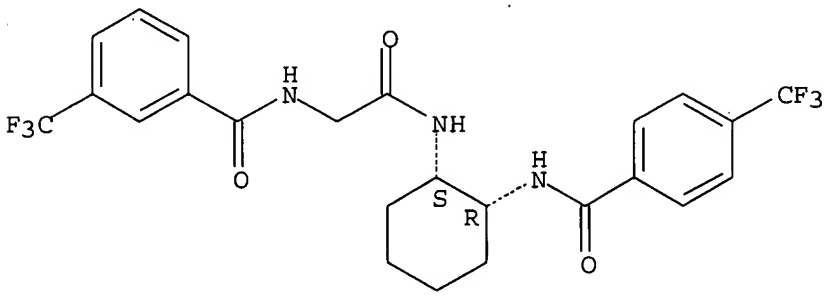
RN 445479-16-3 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[(4-phenoxybenzoyl)amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



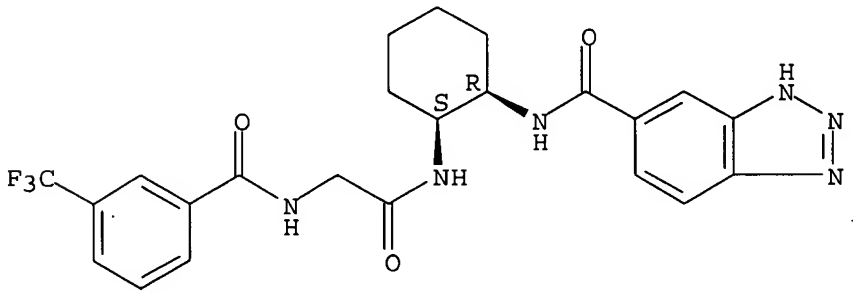
RN 445479-17-4 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(trifluoromethyl)benzoyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



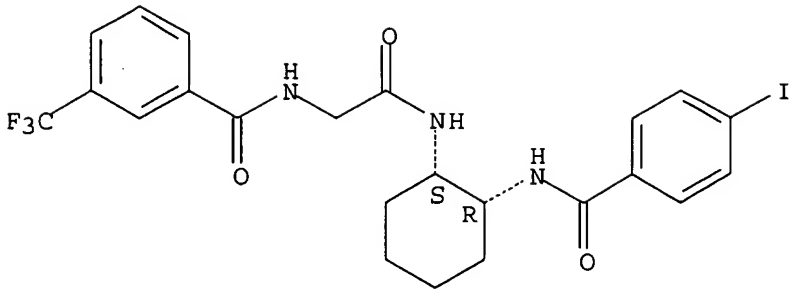
RN 445479-18-5 CAPLUS
CN 1H-Benzotriazole-5-carboxamide, N-[(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



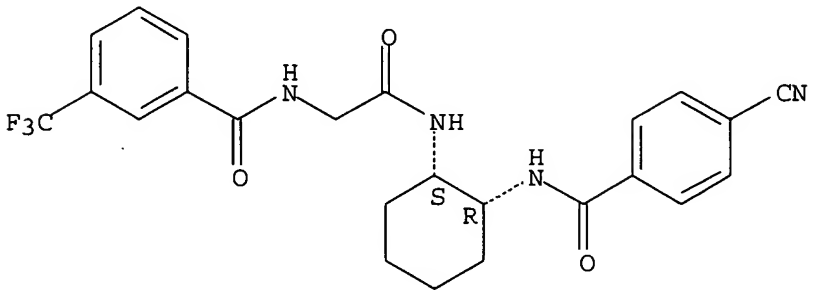
RN 445479-19-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-iodobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



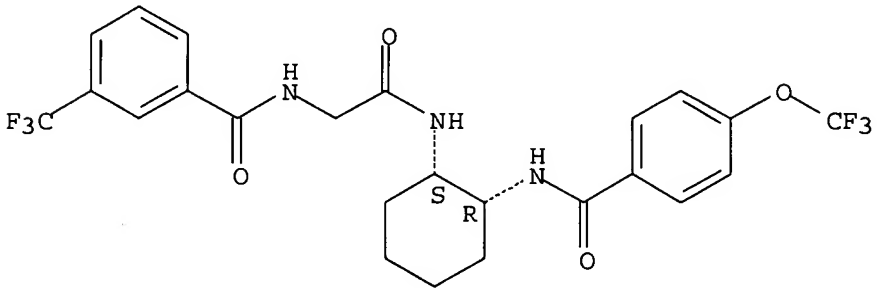
RN 445479-20-9 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-cyanobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



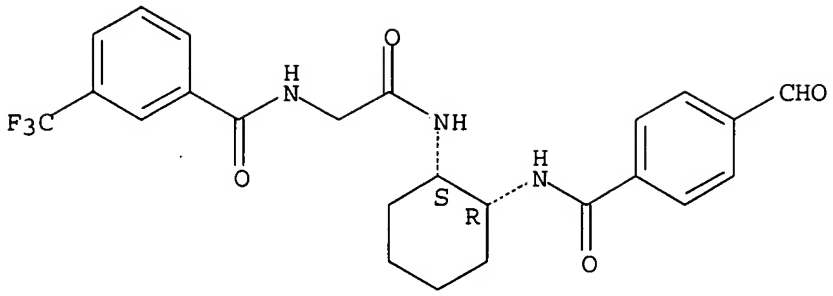
RN 445479-21-0 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(trifluoromethoxy)benzoyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



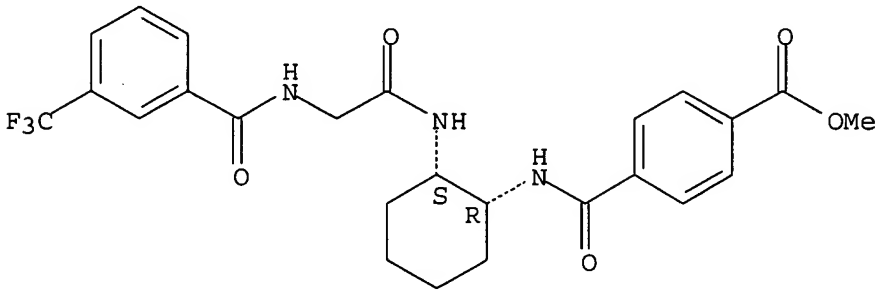
RN 445479-22-1 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-formylbenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



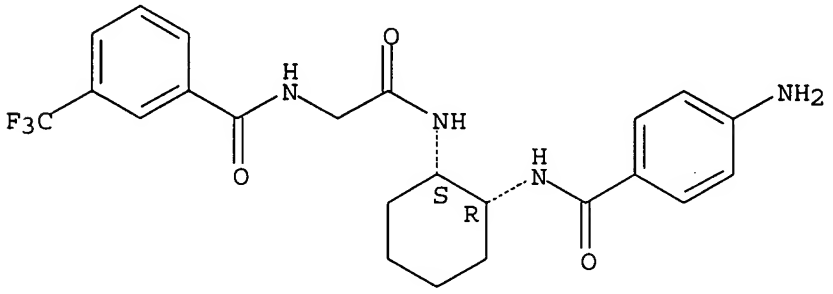
RN 445479-23-2 CAPLUS
CN Benzoic acid, 4-[[[(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]amino]carbonyl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



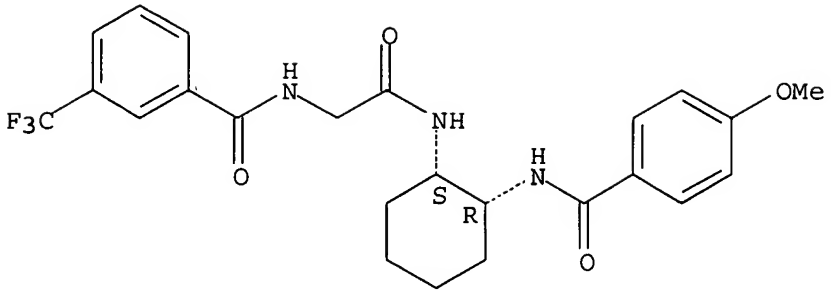
RN 445479-25-4 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-aminobenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



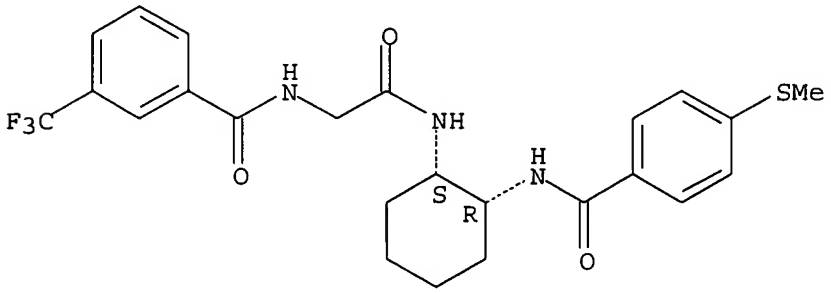
RN 445479-26-5 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[(4-methoxybenzoyl)amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



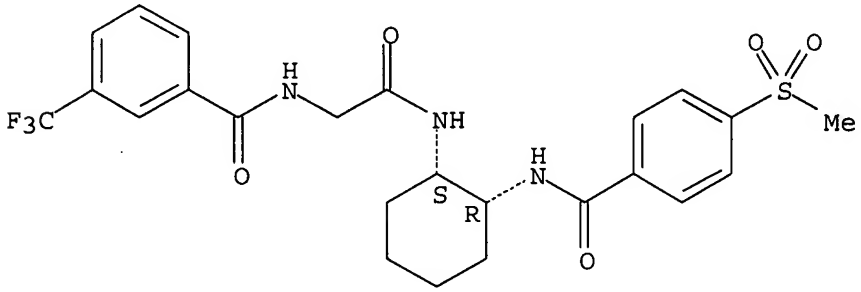
RN 445479-27-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



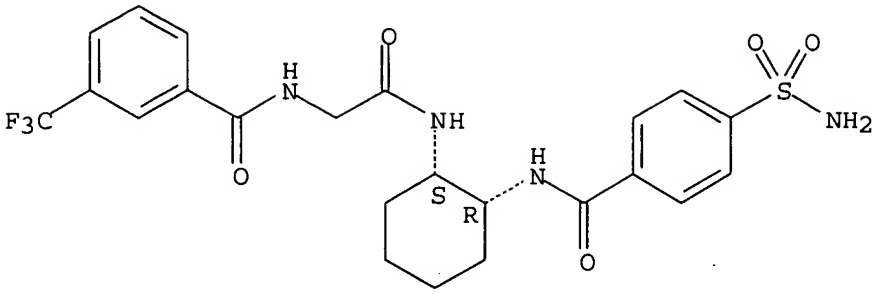
RN 445479-28-7 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



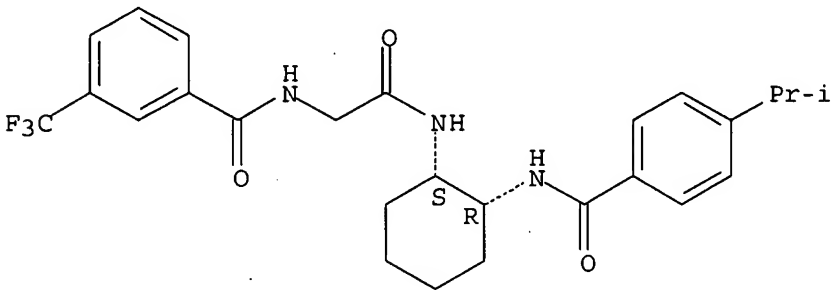
RN 445479-29-8 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



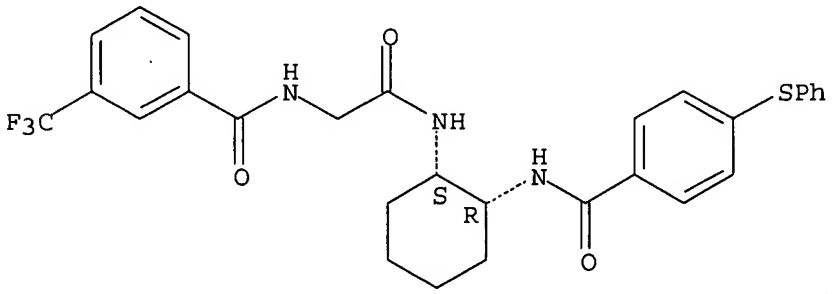
RN 445479-30-1 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(1-methylethyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



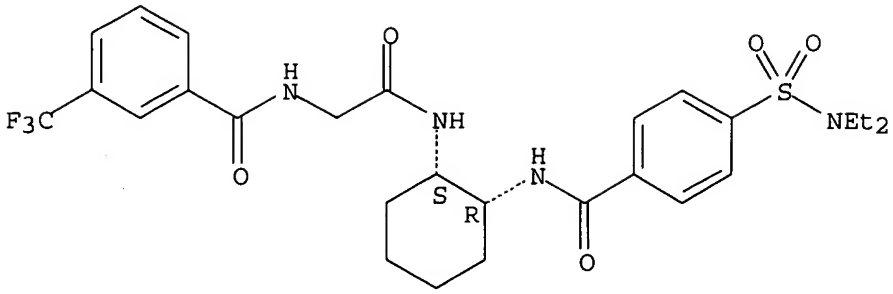
RN 445479-31-2 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-(phenylthio)benzoyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



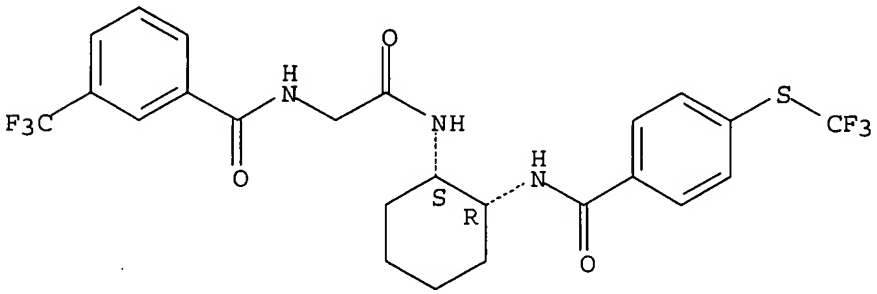
RN 445479-32-3 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-[(diethylamino)sulfonyl]benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



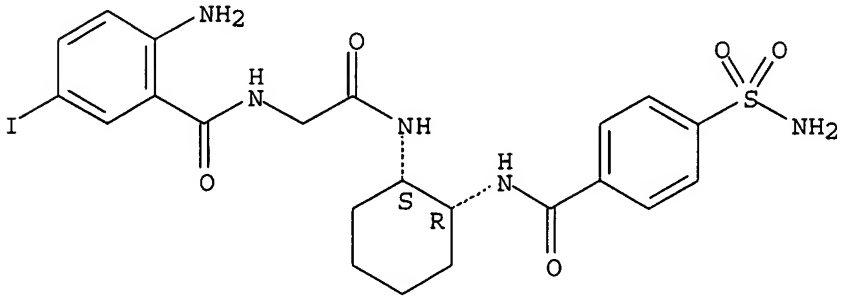
RN 445479-33-4 CAPLUS
CN Benzamide, N-[2-oxo-2-[[(1R,2S)-2-[[4-[(trifluoromethyl)thio]benzoyl]amino]cyclohexyl]amino]ethyl]-3-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



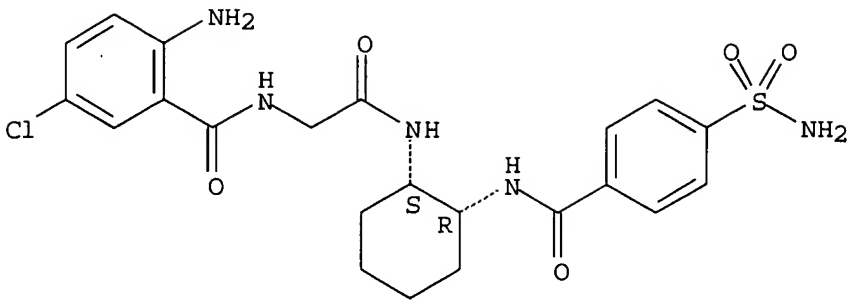
RN 445479-39-0 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodo-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



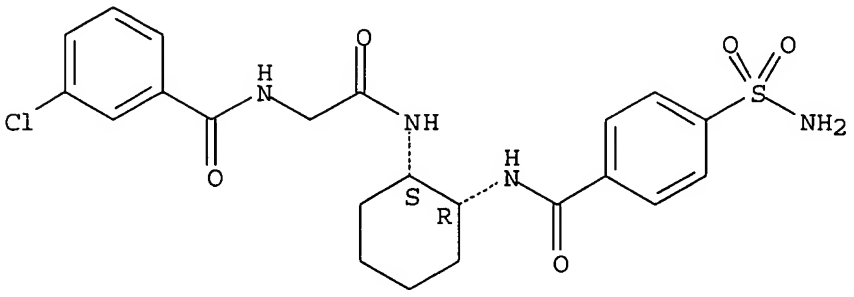
RN 445479-42-5 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-chloro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



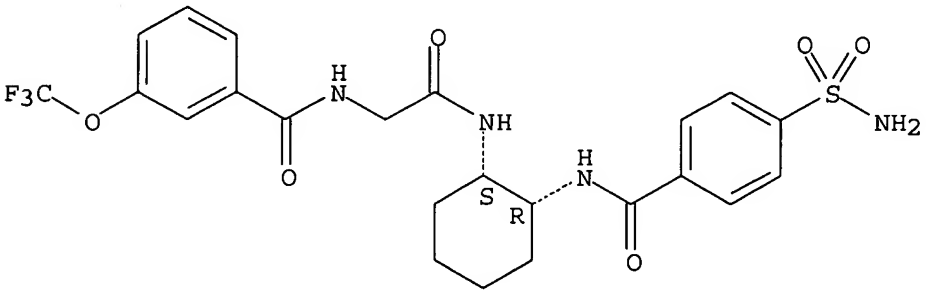
RN 445479-43-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-chloro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



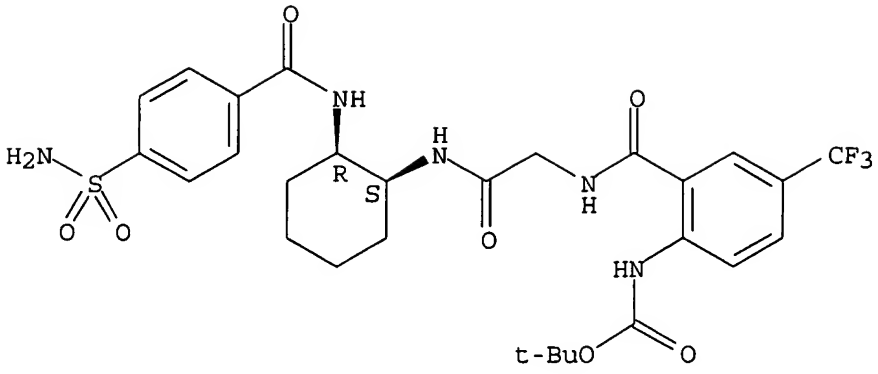
RN 445479-44-7 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethoxy)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



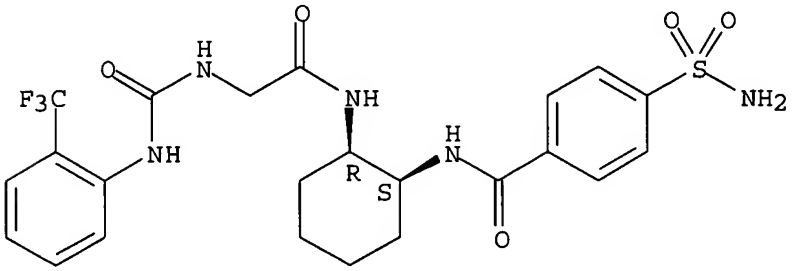
RN 445479-45-8 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



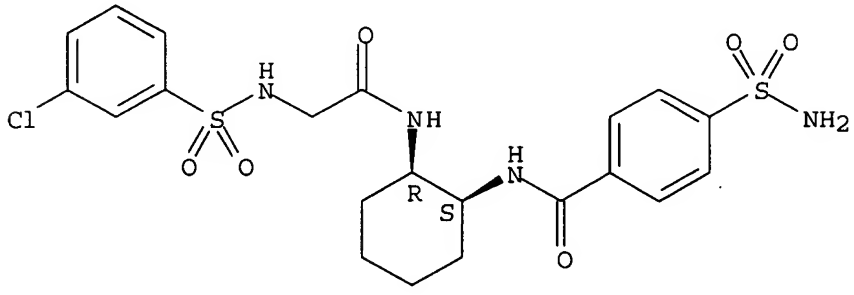
RN 445479-48-1 CAPLUS
CN Benzamide, 4-(aminosulfonyl)-N-[(1R,2S)-2-[[[[[[2-(trifluoromethyl)phenyl]amino]carbonyl]amino]acetyl]amino]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



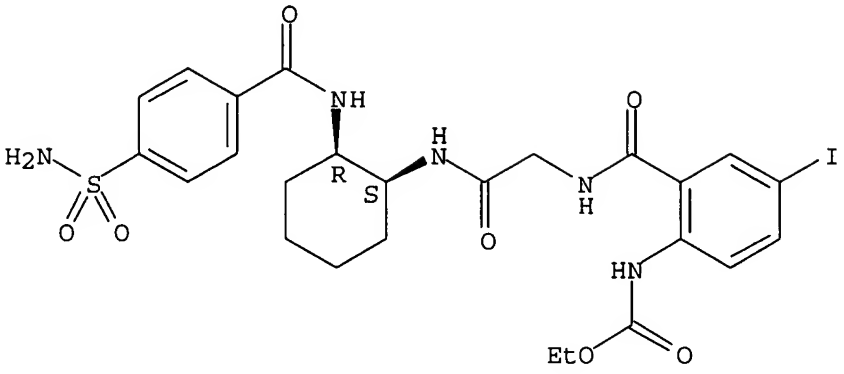
RN 445479-49-2 CAPLUS
CN Benzamide, 4-(aminosulfonyl)-N-[(1R,2S)-2-[[[[(3-chlorophenyl)sulfonyl]amino]acetyl]amino]cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



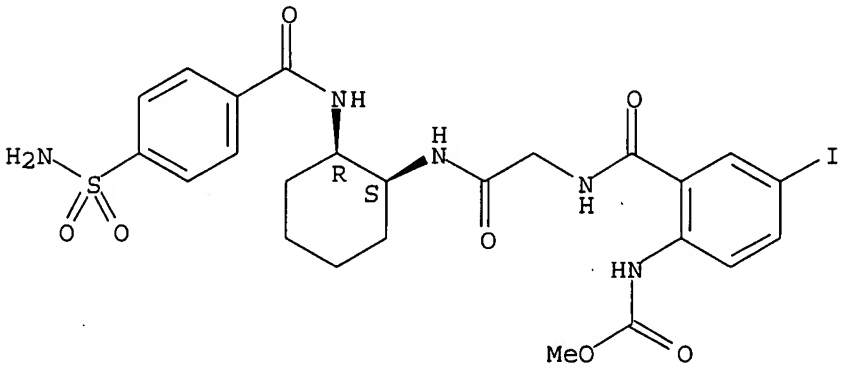
RN 445479-50-5 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



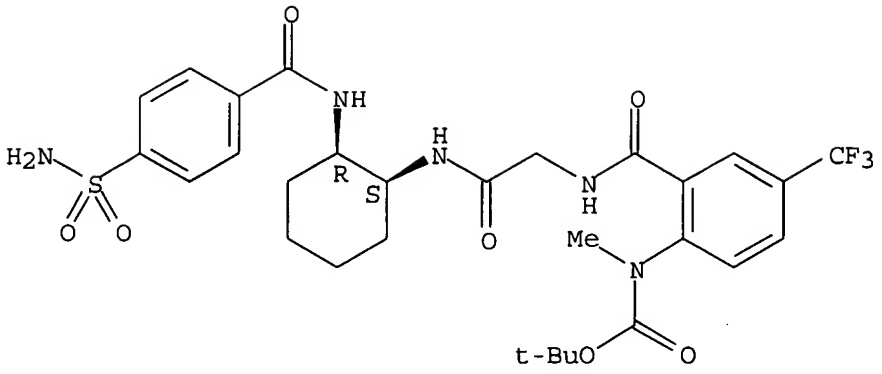
RN 445479-52-7 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



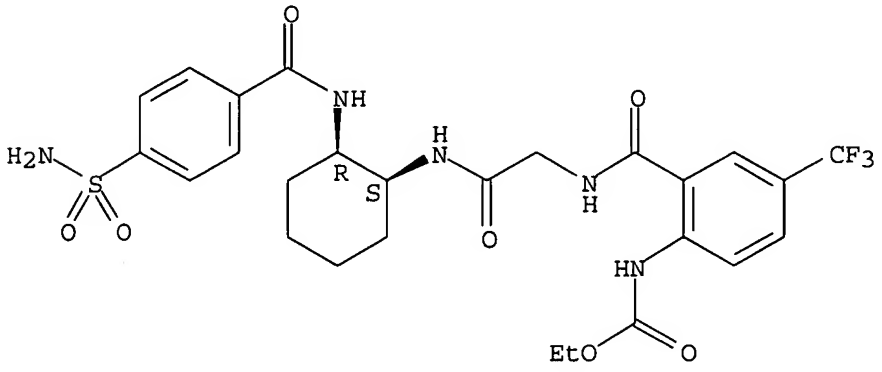
RN 445479-54-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]methyl-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



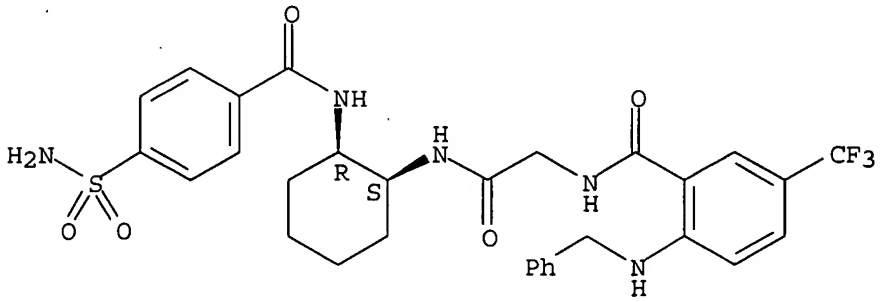
RN 445479-56-1 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cycloh exyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445479-57-2 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]am ino]-2-oxoethyl]-2-[(phenylmethyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

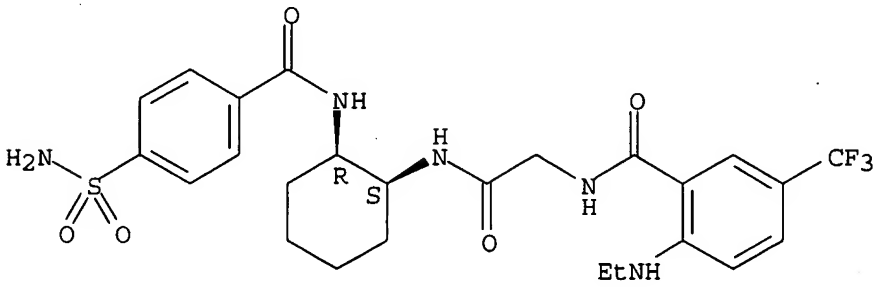
Relative stereochemistry.



RN 445479-58-3 CAPLUS

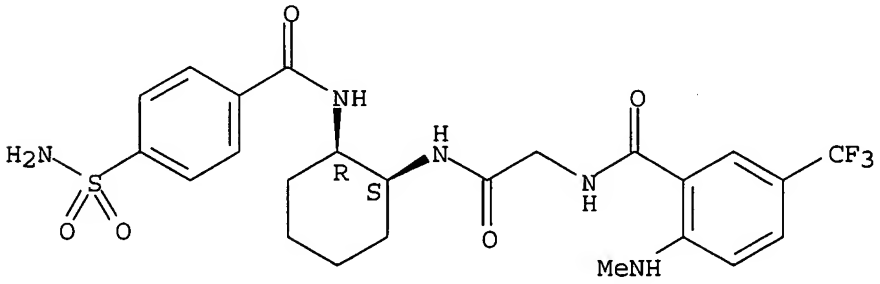
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(ethylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



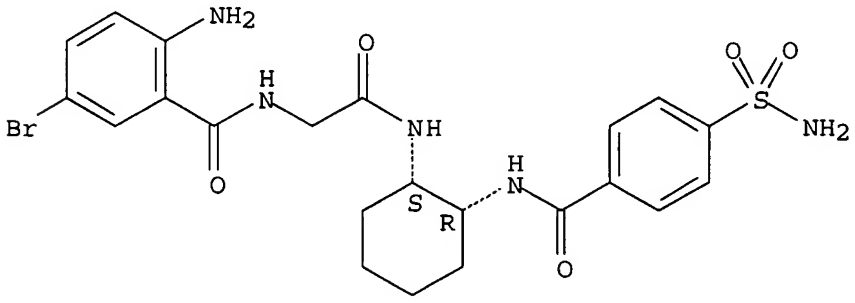
RN 445479-59-4 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(methylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



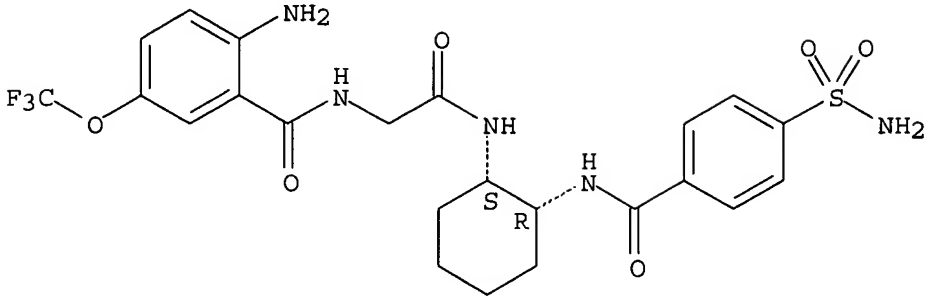
RN 445479-61-8 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-bromo-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



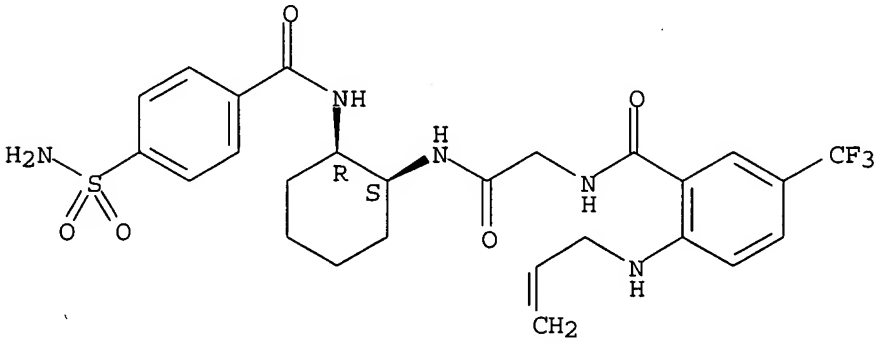
RN 445479-63-0 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethoxy)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



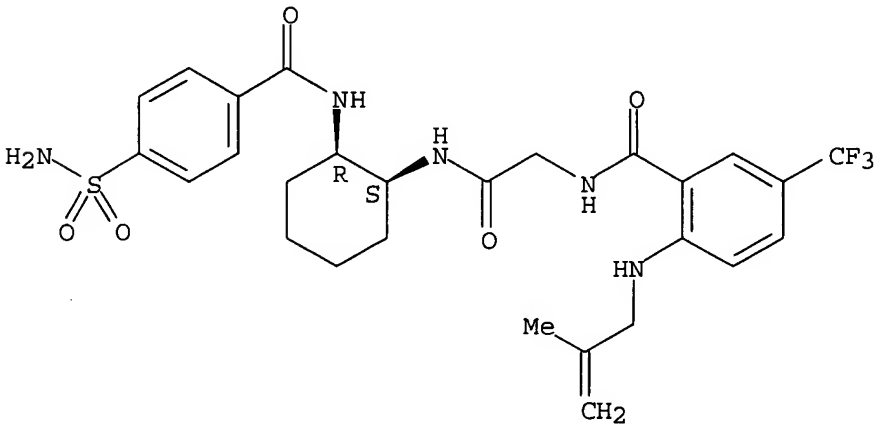
RN 445479-64-1 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(2-propenylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



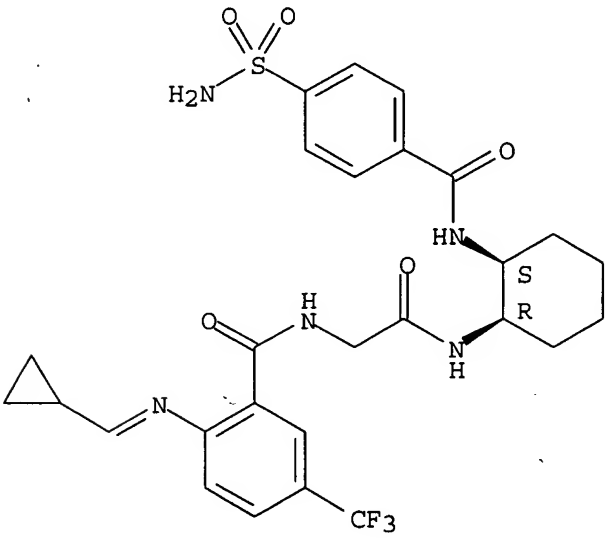
RN 445479-65-2 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



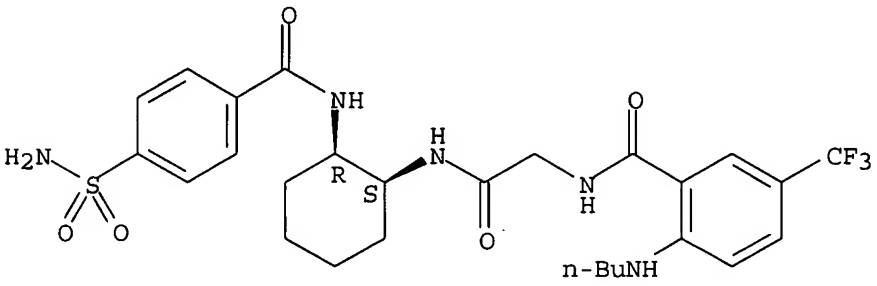
RN 445479-67-4 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(cyclopropylmethylene)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



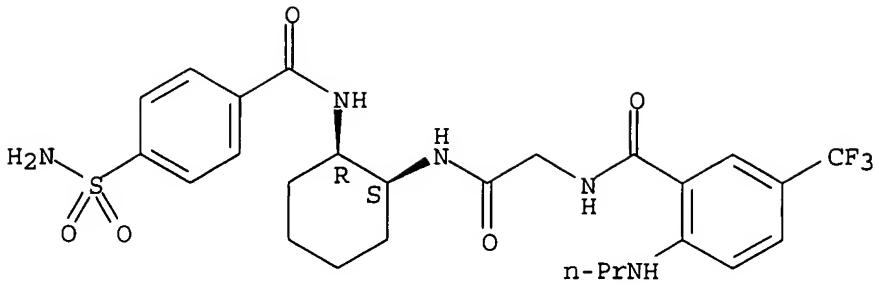
RN 445479-69-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(butylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



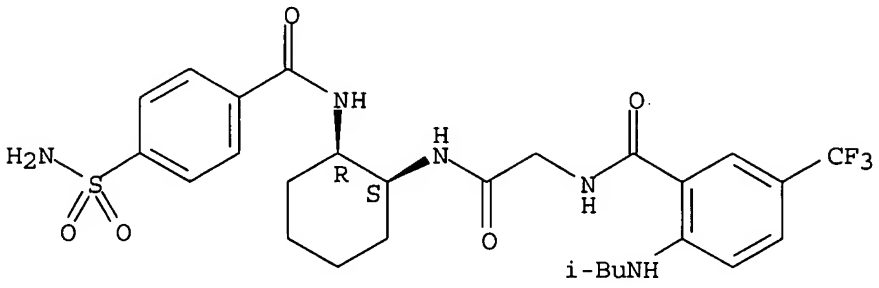
RN 445479-70-9 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(propylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



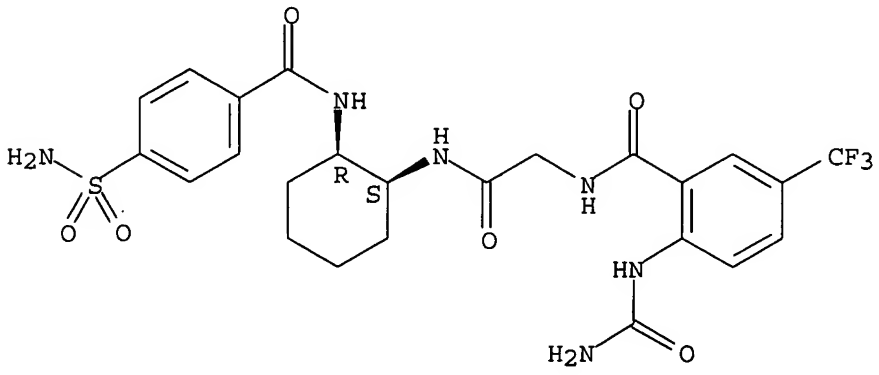
RN 445479-72-1 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(2-methylpropyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



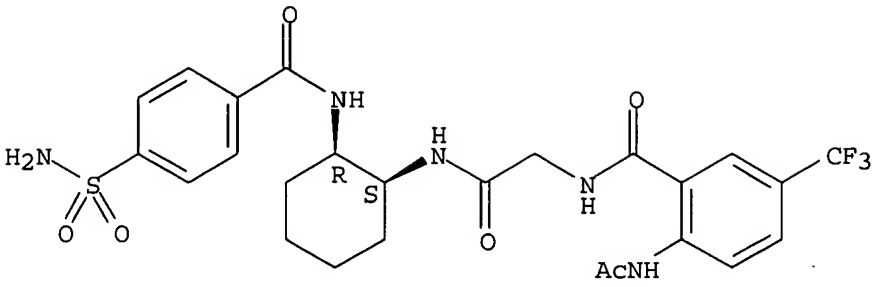
RN 445479-74-3 CAPLUS
CN Benzamide, 2-[(aminocarbonyl)amino]-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



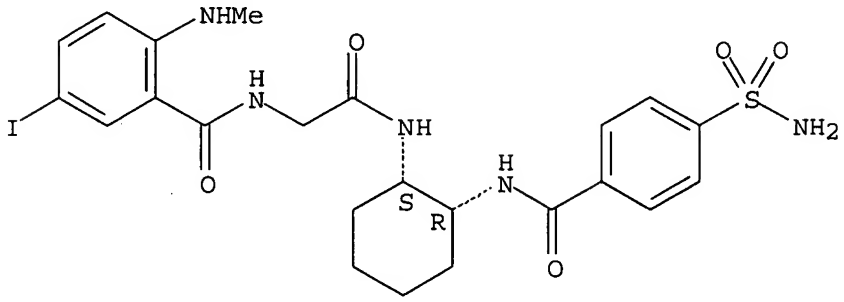
RN 445479-76-5 CAPLUS
CN Benzamide, 2-(acetylamino)-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



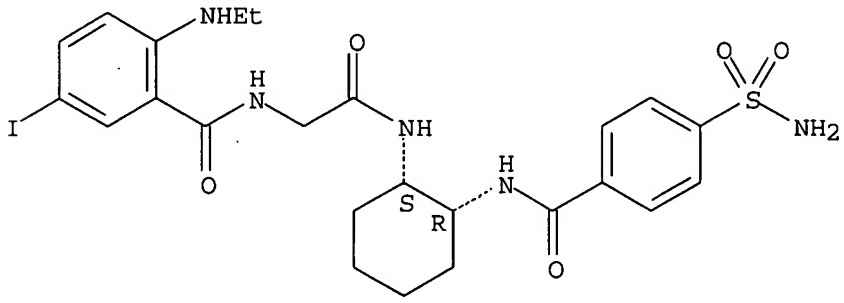
RN 445479-77-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodo-2-(methylamino)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



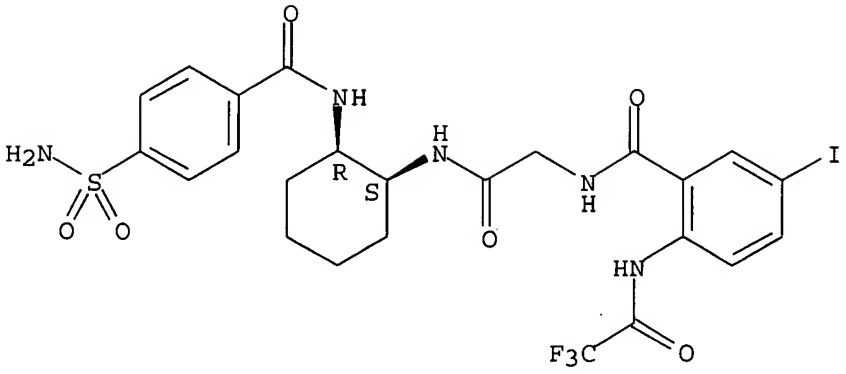
RN 445479-78-7 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(ethylamino)-5-iodo-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



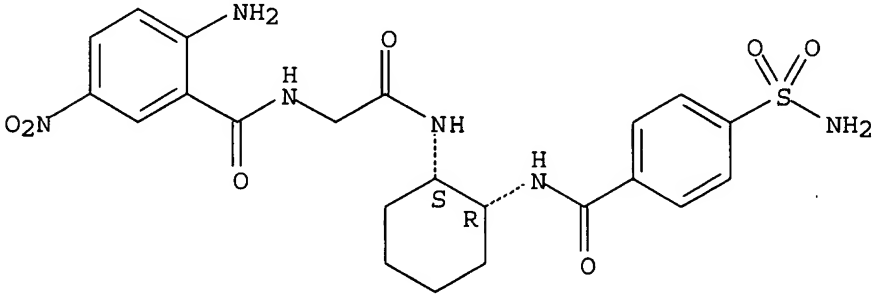
RN 445479-80-1 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-iodo-2-[(trifluoroacetyl)amino]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



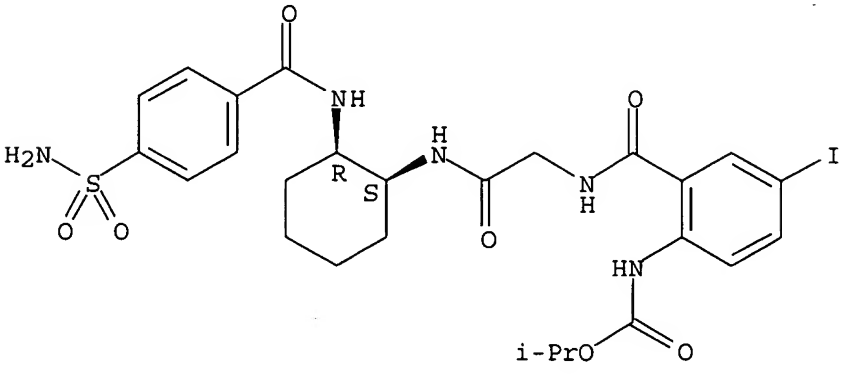
RN 445479-82-3 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-nitro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445479-83-4 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, 1-methylethyl ester, rel- (9CI) (CA INDEX NAME)

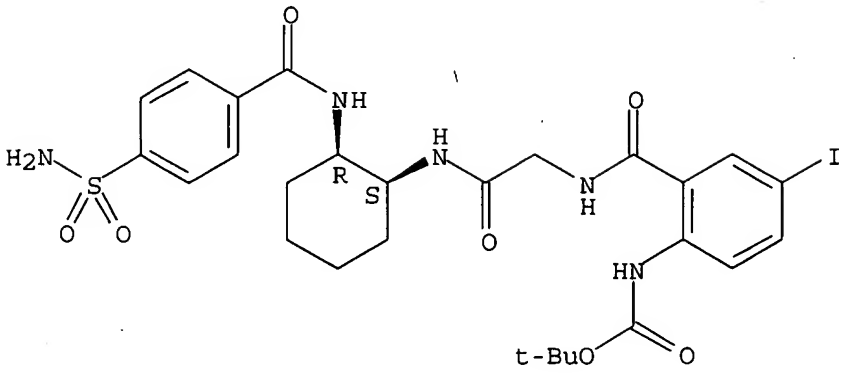
Relative stereochemistry.



RN 445479-85-6 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-iodophenyl]-, 1,1-dimethylethyl

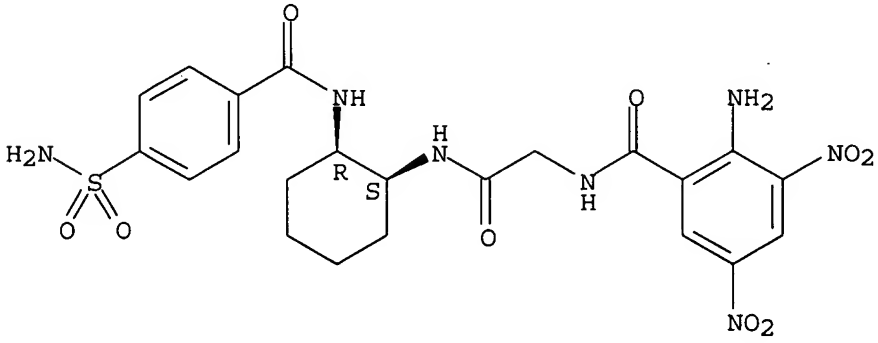
ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



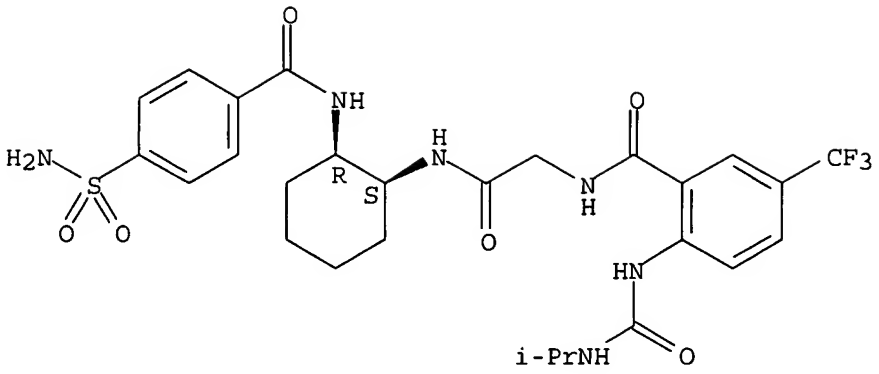
RN 445479-87-8 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3,5-dinitro-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



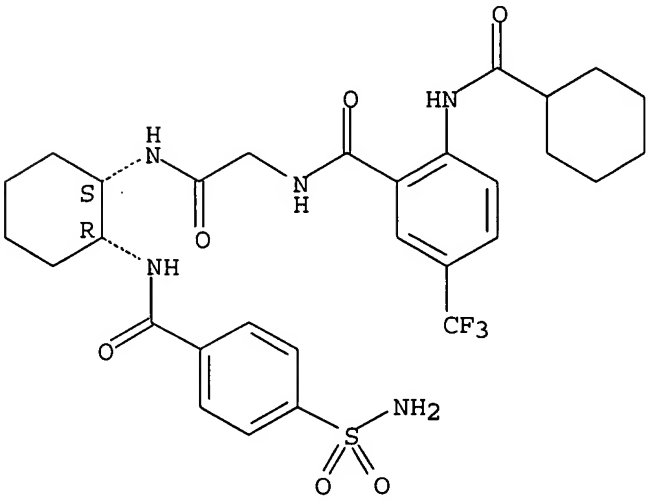
RN 445479-88-9 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



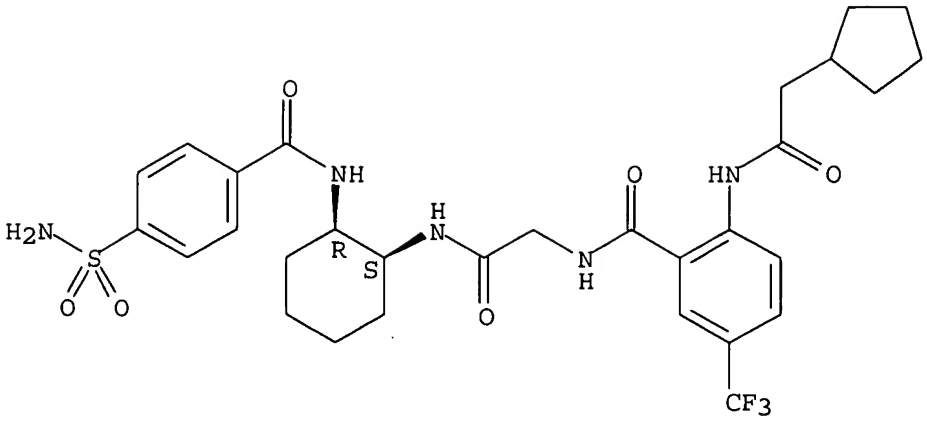
RN 445479-89-0 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(cyclohexylcarbonyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



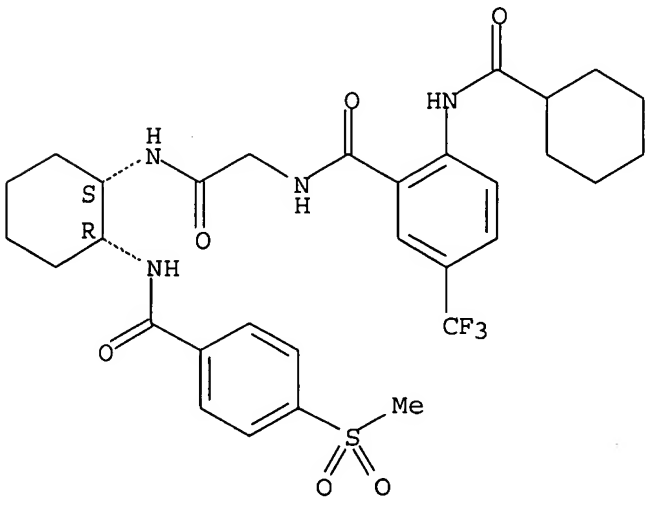
RN 445479-90-3 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(cyclopentylacetyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



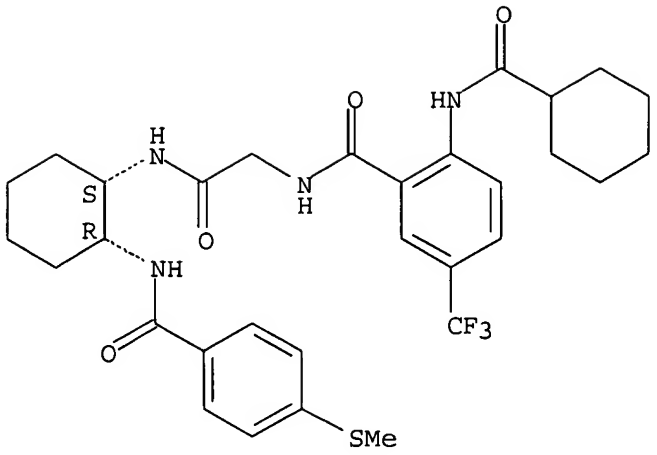
RN 445479-91-4 CAPLUS
CN Benzamide, 2-[(cyclohexylcarbonyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



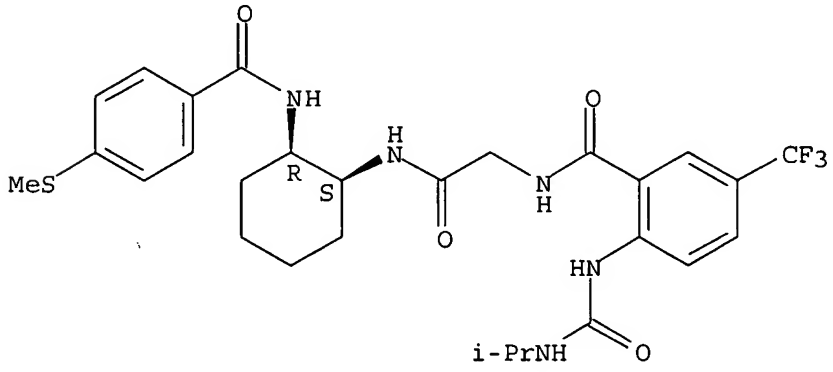
RN 445479-96-9 CAPLUS
CN Benzamide, 2-[(cyclohexylcarbonyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



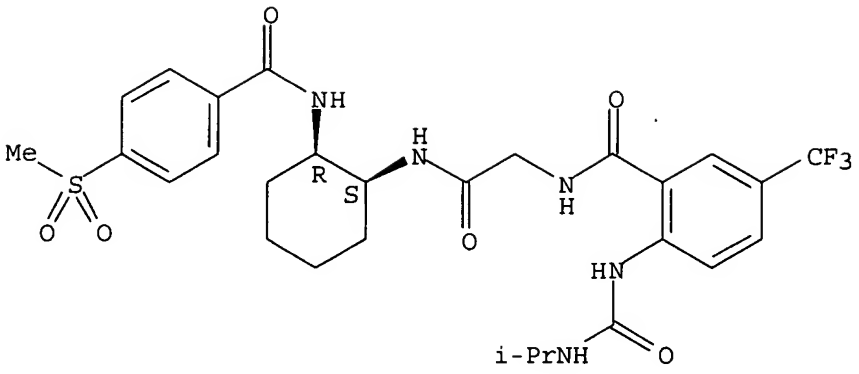
RN 445479-97-0 CAPLUS
CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



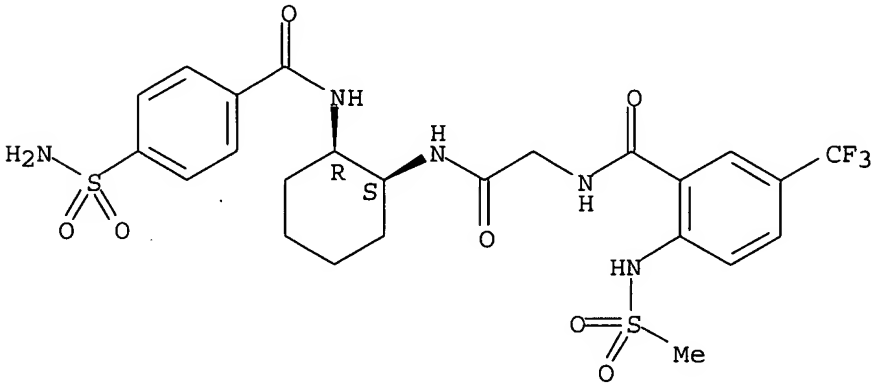
RN 445479-98-1 CAPLUS
CN Benzamide, 2-[[[(1-methylethyl)amino]carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



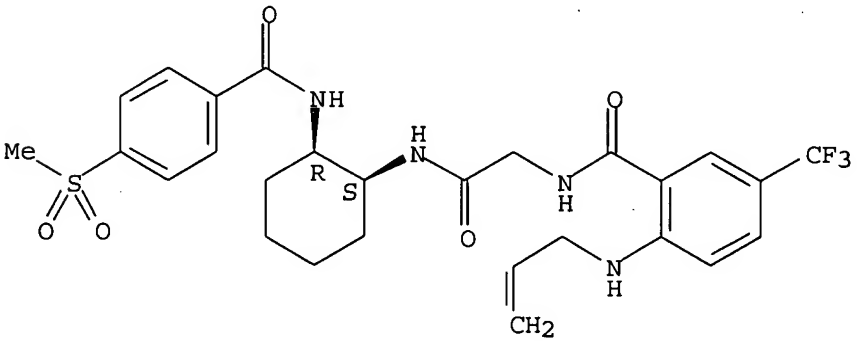
RN 445479-99-2 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[(methylsulfonyl)amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



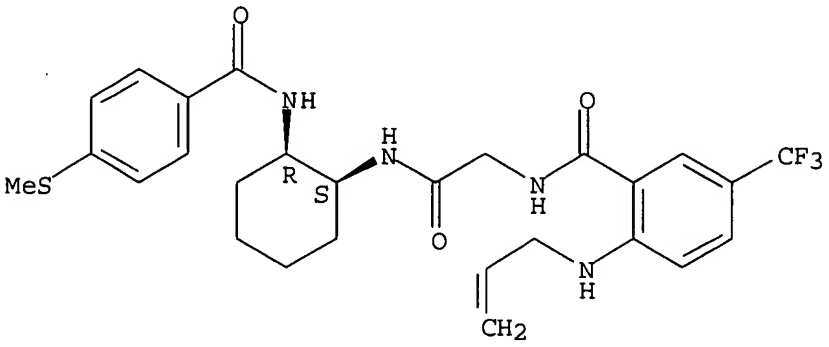
RN 445480-01-3 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(2-propenylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



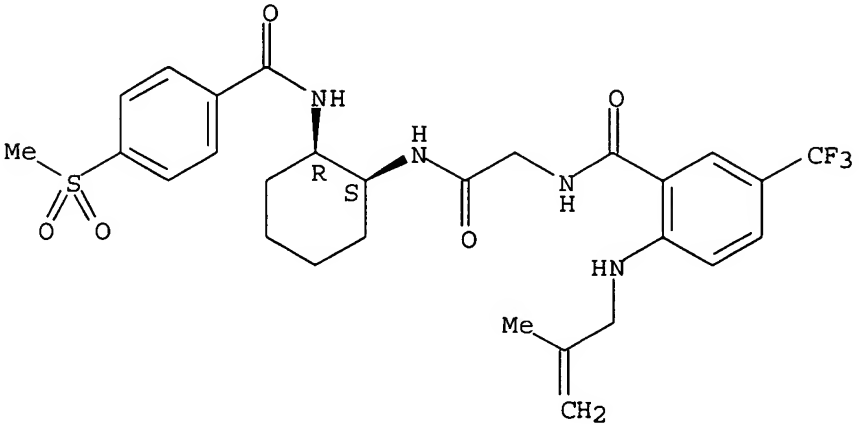
RN 445480-04-6 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(2-propenylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



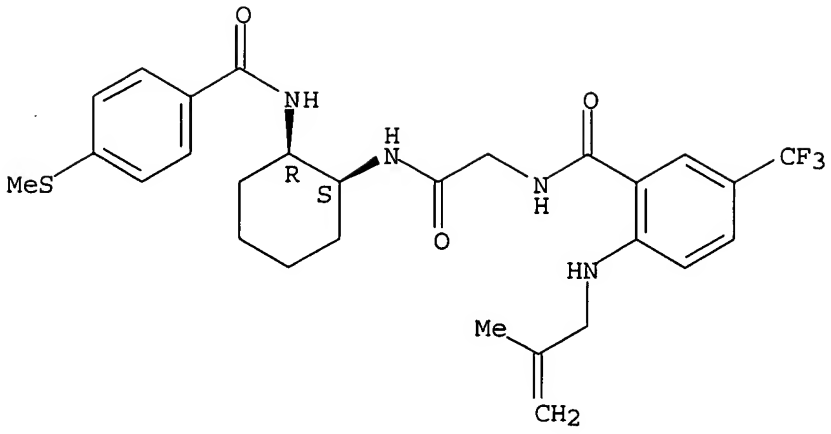
RN 445480-05-7 CAPLUS
CN Benzamide, 2-[(2-methyl-2-propenyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



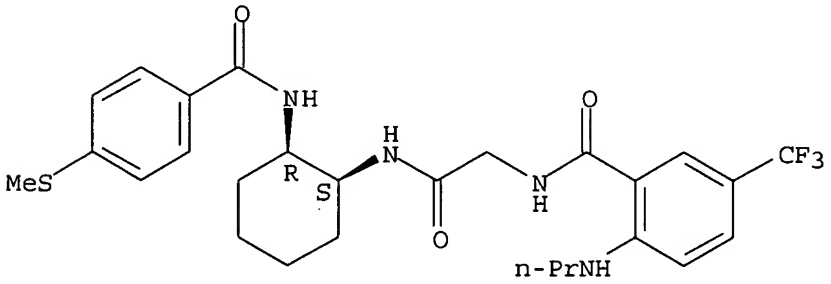
RN 445480-06-8 CAPLUS
CN Benzamide, 2-[(2-methyl-2-propenyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



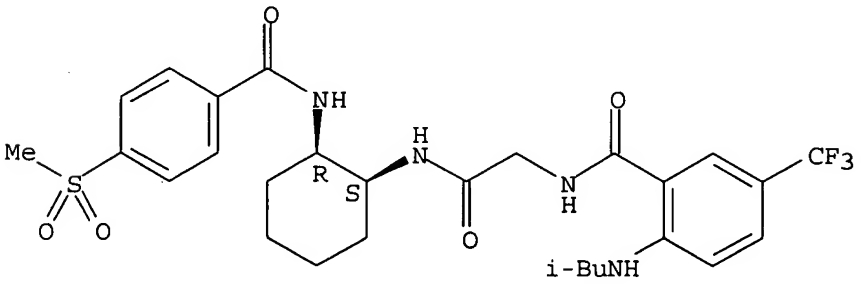
RN 445480-08-0 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-(propylamino)-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445480-09-1 CAPLUS
CN Benzamide, 2-[(2-methylpropyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

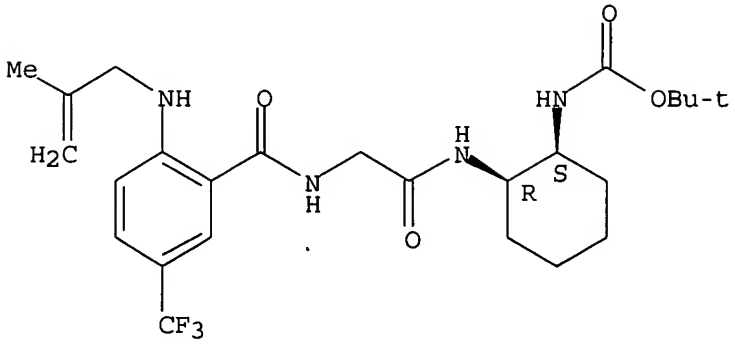
Relative stereochemistry.



RN 445480-10-4 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[2-[(2-methyl-2-propenyl)amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-,

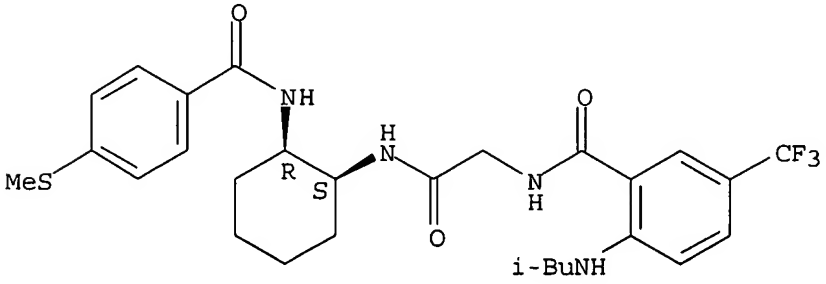
1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



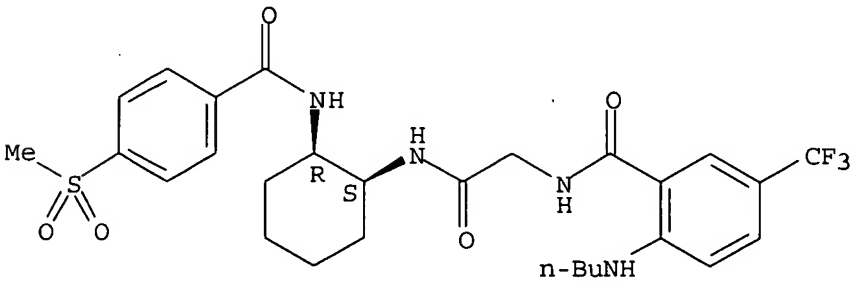
RN 445480-11-5 CAPLUS
CN Benzamide, 2-[(2-methylpropyl)amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445480-12-6 CAPLUS
CN Benzamide, 2-(butylamino)-N-[2-[[(1R,2S)-2-[[4-(methylsulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

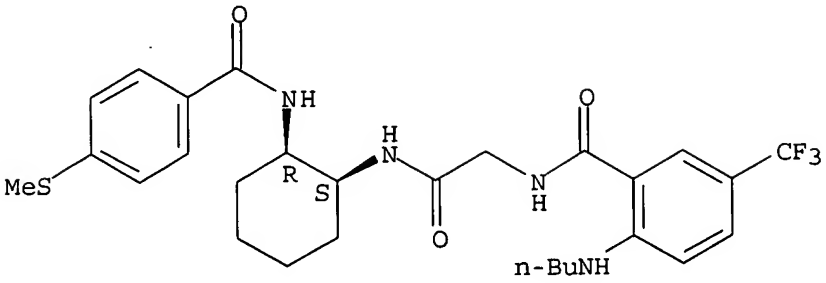
Relative stereochemistry.



RN 445480-13-7 CAPLUS
CN Benzamide, 2-(butylamino)-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-

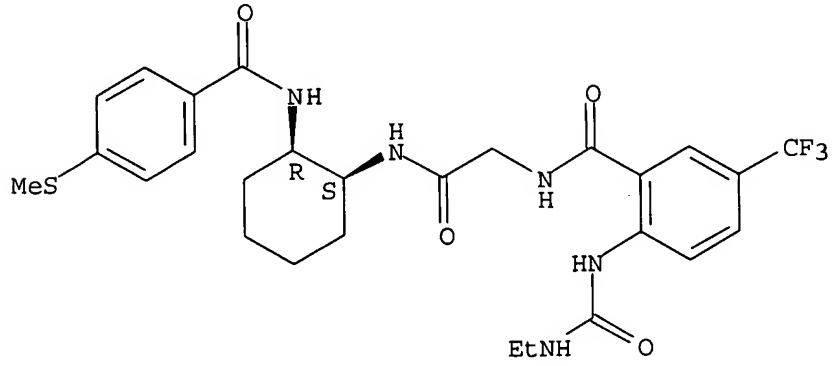
(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



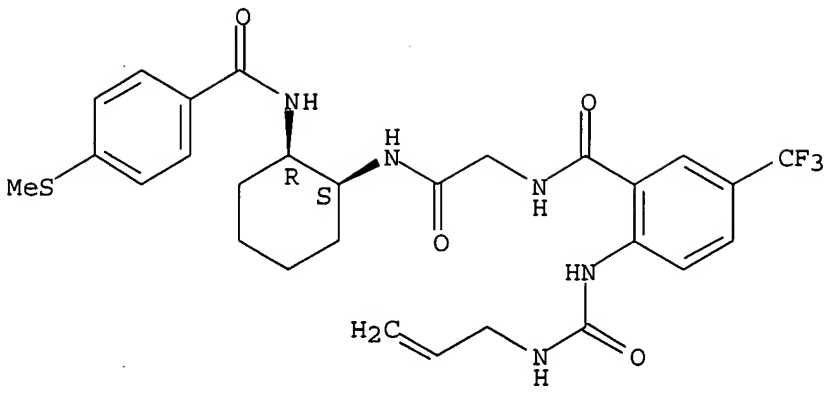
RN 445480-14-8 CAPLUS
CN Benzamide, 2-[[(ethylamino)carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



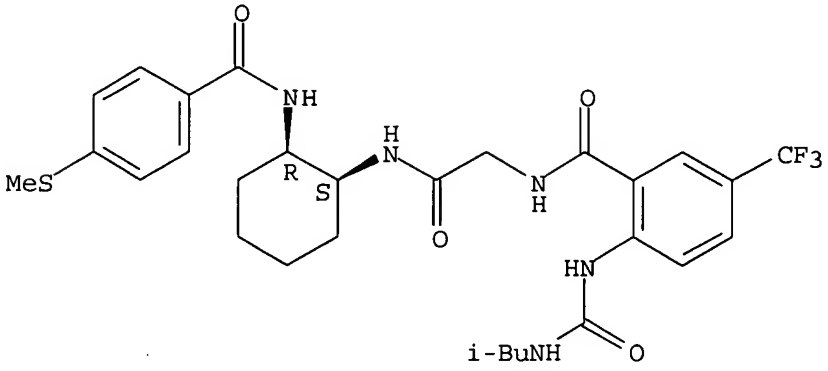
RN 445480-16-0 CAPLUS
CN Benzamide, N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-2-[[(2-propenylamino)carbonyl]amino]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



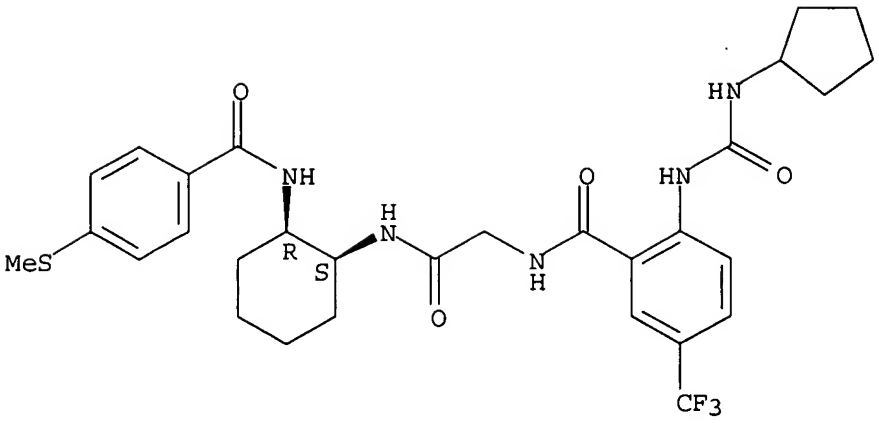
RN 445480-18-2 CAPLUS
CN Benzamide, 2-[[[(2-methylpropyl)amino]carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



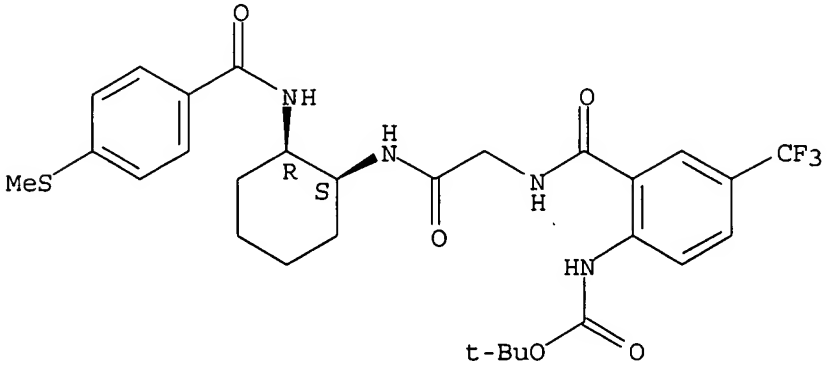
RN 445480-21-7 CAPLUS
CN Benzamide, 2-[[(cyclopentylamino)carbonyl]amino]-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



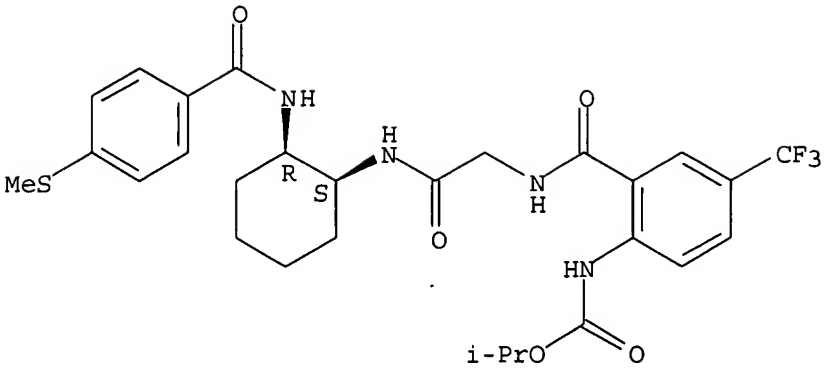
RN 445480-23-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



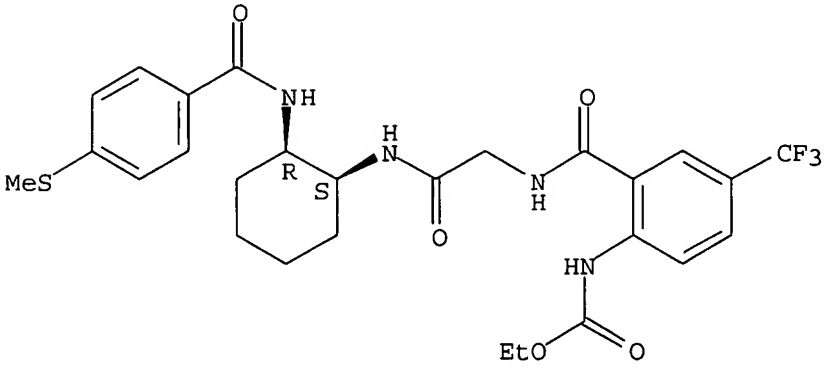
RN 445480-24-0 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1-methylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



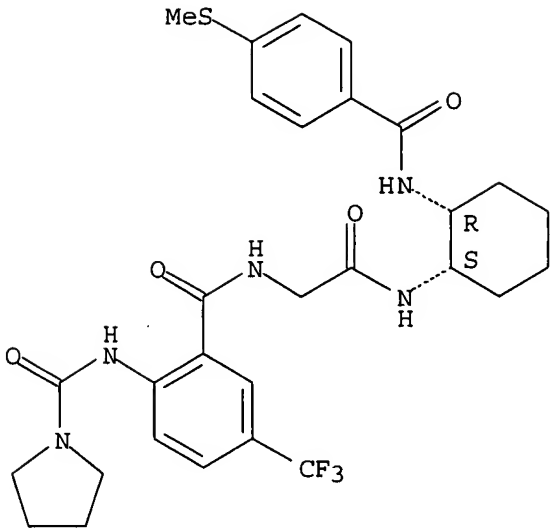
RN 445480-26-2 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



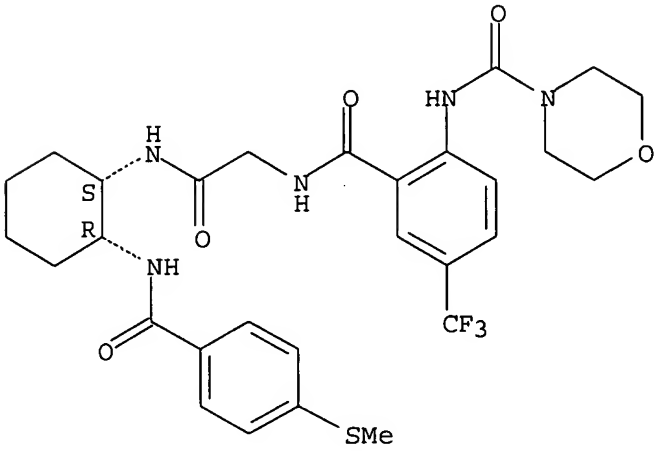
RN 445480-28-4 CAPLUS
CN 1-Pyrrolidinecarboxamide, N-[2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



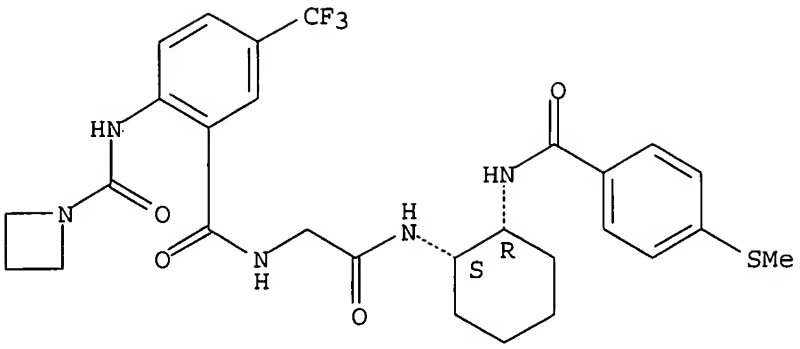
RN 445480-29-5 CAPLUS
CN 4-Morpholinecarboxamide, N-[2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

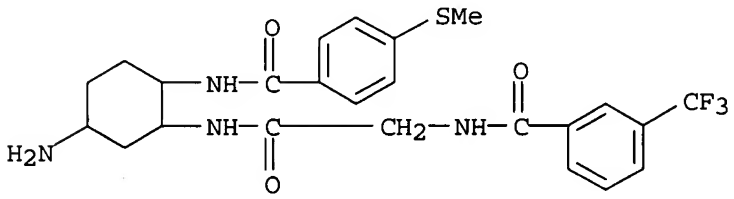


RN 445480-31-9 CAPLUS
CN 1-Azetidinecarboxamide, N-[2-[[[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, rel- (9CI) (CA INDEX NAME)

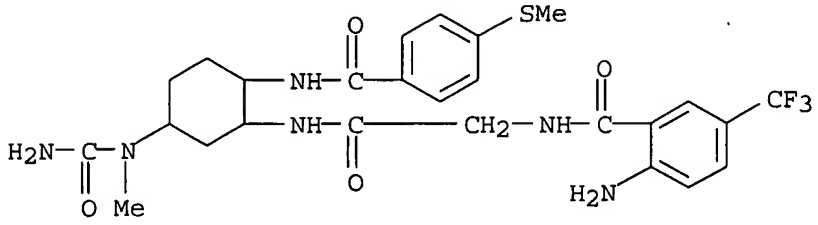
Relative stereochemistry.



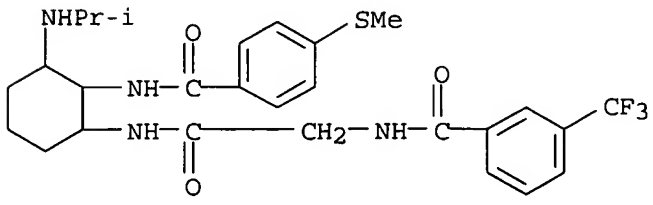
RN 445480-48-8 CAPLUS
CN Benzamide, N-[2-[[5-amino-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



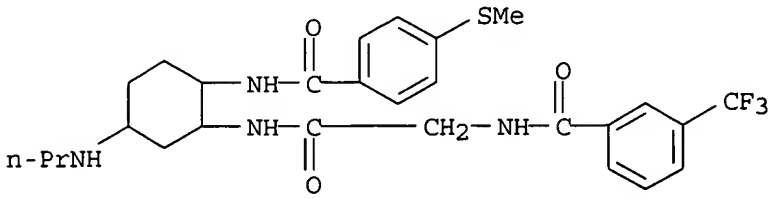
RN 445480-53-5 CAPLUS
CN Benzamide, 2-amino-N-[2-[[5-[(aminocarbonyl)methylamino]-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



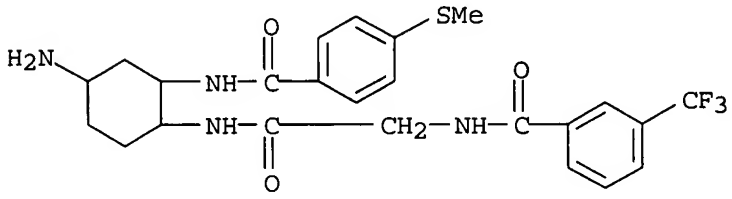
RN 445480-57-9 CAPLUS
CN Benzamide, N-[2-[[3-[(1-methylethyl)amino]-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 445480-67-1 CAPLUS
CN Benzamide, N-[2-[[2-[[4-(methylthio)benzoyl]amino]-5-(propylamino)cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

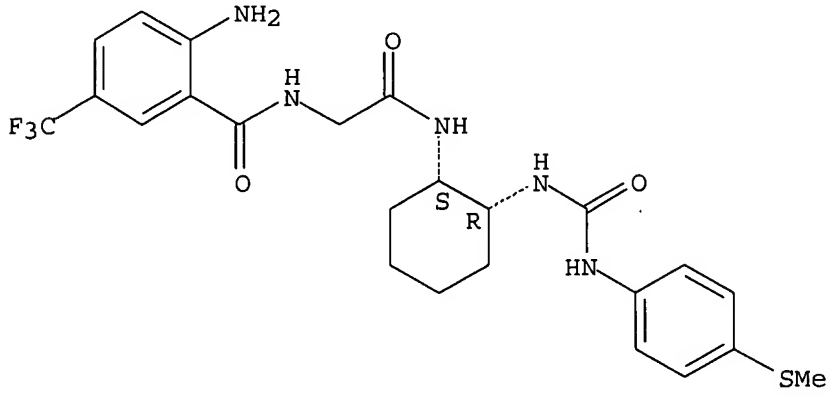


RN 445480-68-2 CAPLUS
CN Benzamide, N-[2-[[4-amino-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



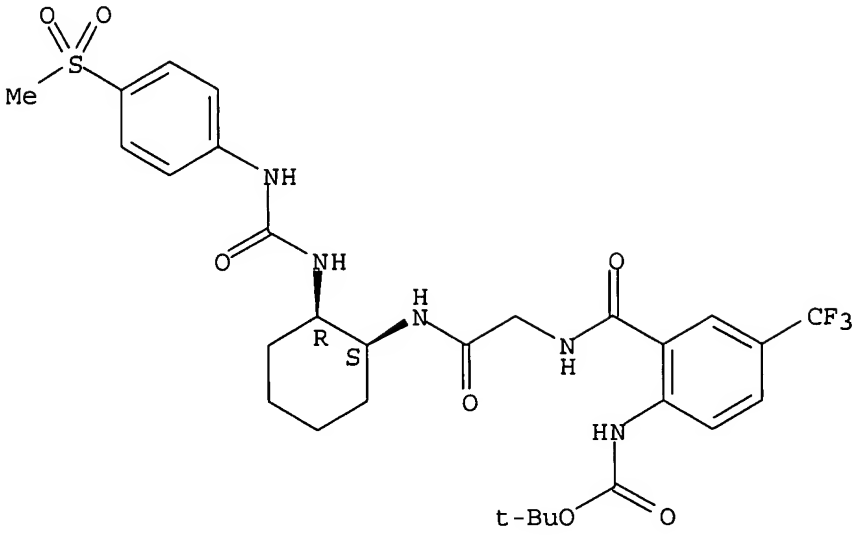
RN 445481-22-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[[[4-(methylthio)phenyl]amino]carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445481-23-2 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1R,2S)-2-[[[[4-(methylsulfonyl)phenyl]amino]carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



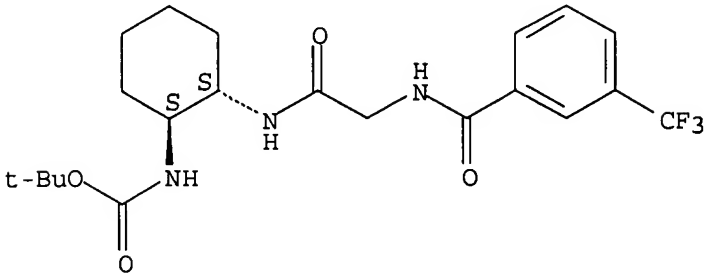
IT **445478-72-8P**, [(1S,2S)-2-[[[[3-(Trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]carbamic acid 1,1-dimethylethyl ester **445479-11-8P**, [cis-2-[[[[3-(Trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]carbamic acid 1,1-dimethylethyl ester **445479-40-3P**, Benzyl cis-[2-[[2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]carbamate **445479-41-4P**, N-cis-[2-[(Aminoacetyl)amino]cyclohexyl]-4-(aminosulfonyl)benzamide hydrobromide **445479-93-6P 445479-94-7P**, [cis-2-[[[[[2-(tert-Butyloxycarbonylamino)-5-trifluoromethyl]benzoyl]amino]acetyl]amino]cyclohexyl]carbamic acid benzyl ester **445480-02-4P 445480-03-5P 445480-15-9P**, 2-(Amino)-N-[2-[[cis-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)benzamide **445480-20-6P 445480-55-7P**, [5-Benzyloxycarbonylamino-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid tert-butyl ester **445480-56-8P**, [3-(4-Methylthiobenzoylamino)-4-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid benzyl ester **445480-63-7P**, [4-Benzyloxycarbonylamino-2-[2-[((2-(tert-butoxycarbonylamino)-5-(trifluoromethyl)benzoyl)amino)acetyl]amino]cyclohexyl]carbamic acid tert-butyl ester **445480-65-9P**, [3-[[2-(2-Amino-5-trifluoromethylbenzoylamino)acetyl]amino]-4-(4-methylsulfanylbenzoylamino)cyclohexyl]carbamic acid benzyl ester **445480-66-0P**, [4-Benzyloxycarbonylamino-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid tert-butyl ester **445480-71-7P**, cis-[2-[[2-(2-Isopropylamino-5-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid tert-butyl ester **445480-73-9P 445480-75-1P 445481-13-0P**, [5-Benzyloxy-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid tert-butyl ester **445481-14-1P**, [5-Azido-2-[[2-(3-trifluoromethylbenzoylamino)acetyl]amino]cyclohexyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of [(cycloalkylamino)oxoethyl]benzamides and related compds. as modulators of chemokine receptor activity)

RN 445478-72-8 CAPLUS

CN Carbamic acid, [(1S,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amin

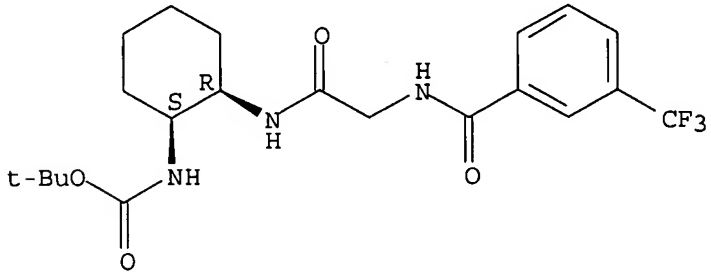
o]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



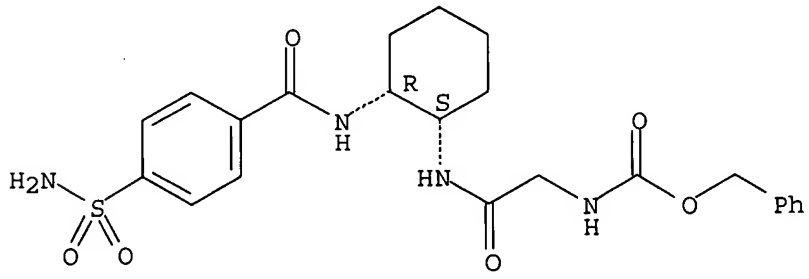
RN 445479-11-8 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amin
o]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



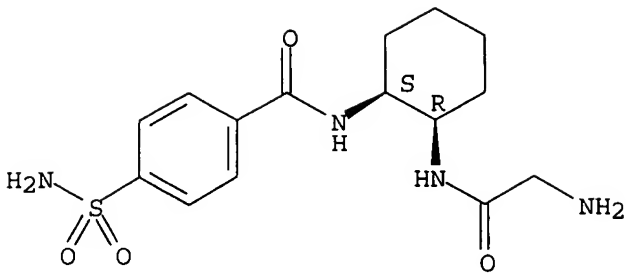
RN 445479-40-3 CAPLUS
CN Carbamic acid, [2-[[(1R,2S)-2-[[4-(aminosulfonyl)benzoyl]amino]cyclohexyl]
amino]-2-oxoethyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 445479-41-4 CAPLUS
CN Benzamide, N-[(1R,2S)-2-[(aminoacetyl)amino]cyclohexyl]-4-(aminosulfonyl)-
, monohydrobromide, rel- (9CI) (CA INDEX NAME)

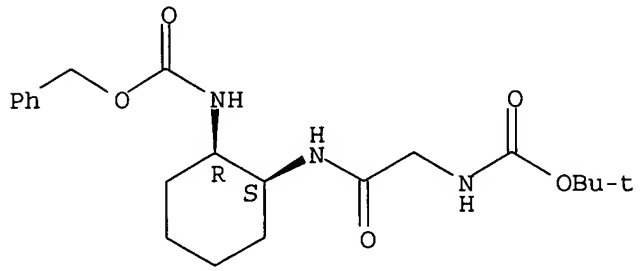
Relative stereochemistry.



● HBr

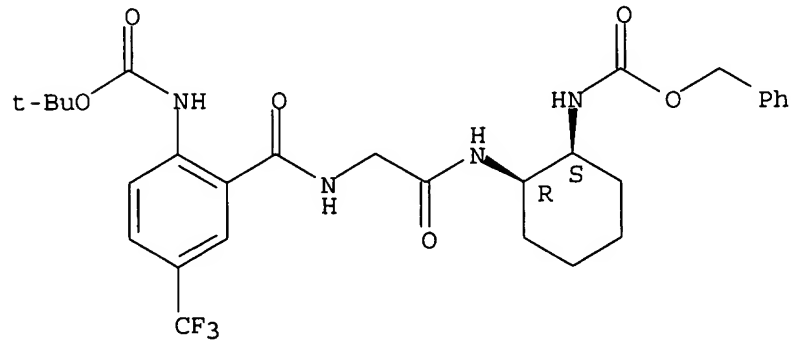
RN 445479-93-6 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



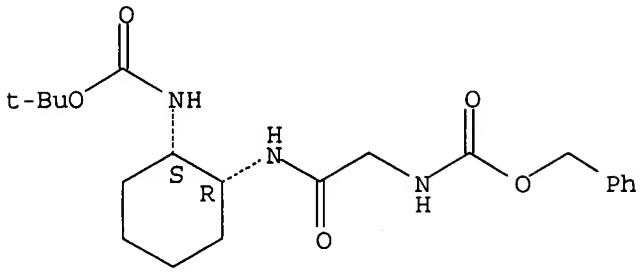
RN 445479-94-7 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



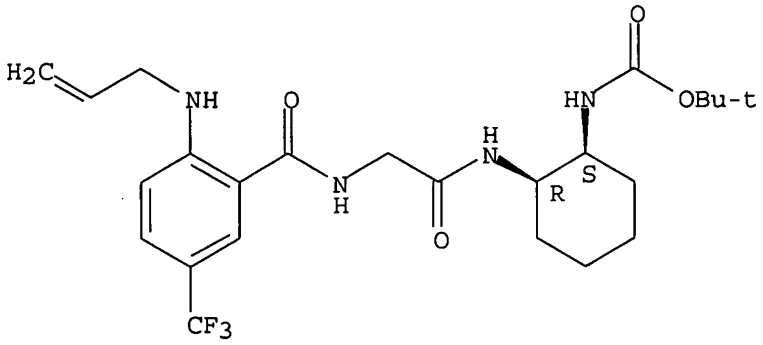
RN 445480-02-4 CAPLUS
CN Carbamic acid, [2-[[(1R,2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]cyclohexyl]amino]-2-oxoethyl]-, phenylmethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



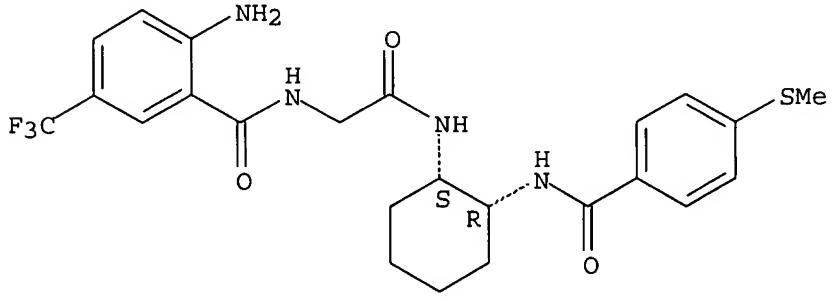
RN 445480-03-5 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[2-(2-propenylamino)-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



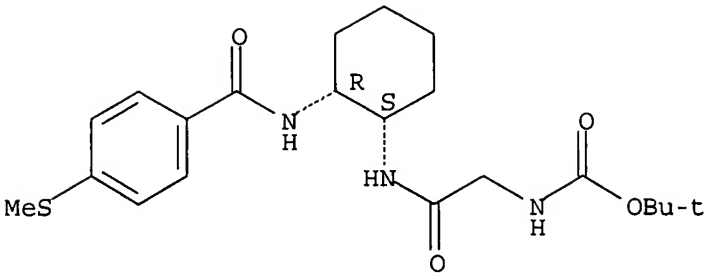
RN 445480-15-9 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-5-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

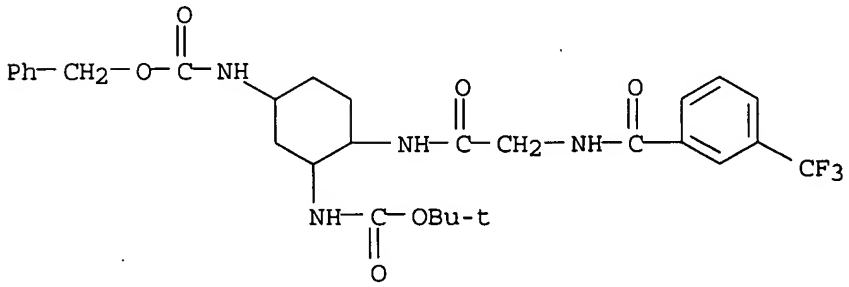


RN 445480-20-6 CAPLUS
CN Carbamic acid, [2-[[(1R,2S)-2-[[4-(methylthio)benzoyl]amino]cyclohexyl]amino]-2-oxoethyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

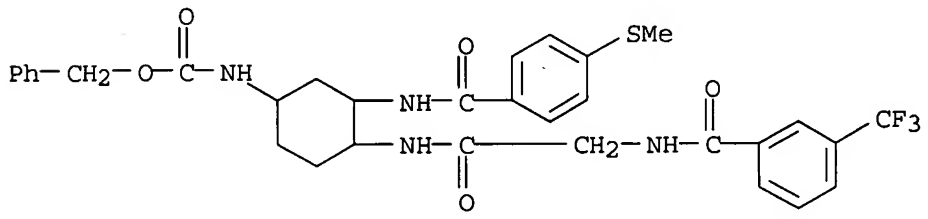
Relative stereochemistry.



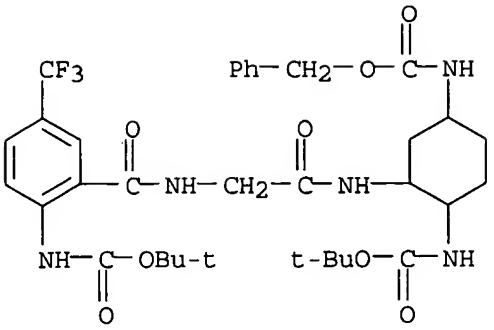
RN 445480-55-7 CAPLUS
CN Carbamic acid, [3-[[(1,1-dimethylethoxy)carbonyl]amino]-4-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



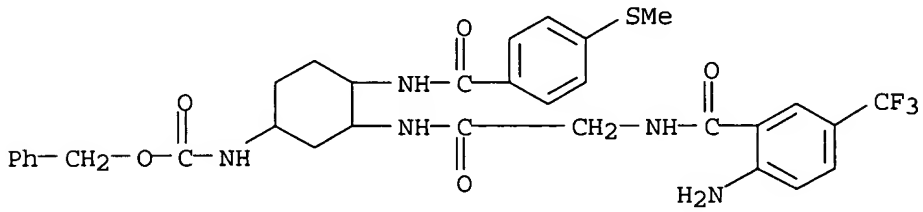
RN 445480-56-8 CAPLUS
CN Carbamic acid, [3-[[4-(methylthio)benzoyl]amino]-4-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



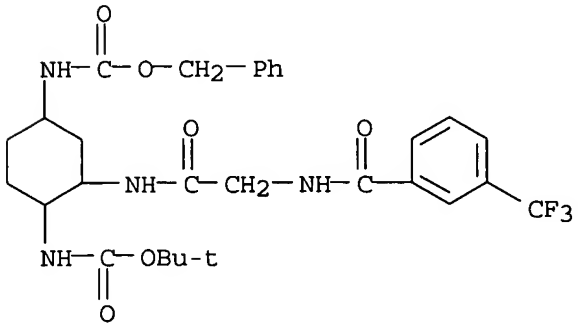
RN 445480-63-7 CAPLUS
CN Carbamic acid, [4-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 445480-65-9 CAPLUS
CN Carbamic acid, [3-[[[[2-amino-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-4-[[4-(methylthio)benzoyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

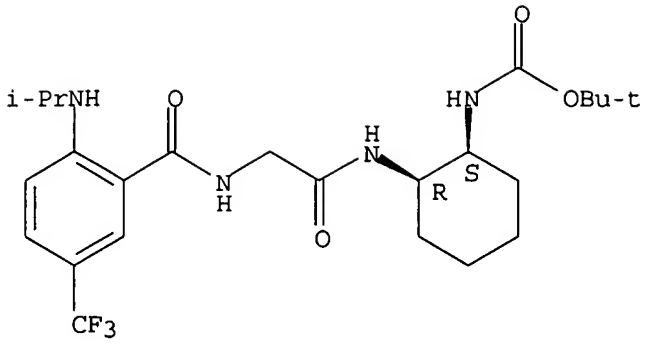


RN 445480-66-0 CAPLUS
CN Carbamic acid, [4-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



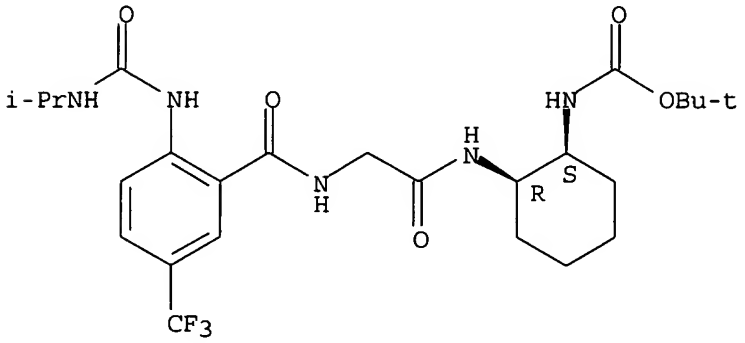
RN 445480-71-7 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[2-[(1-methylethyl)amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

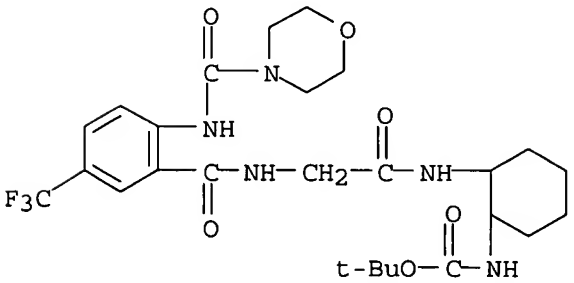


RN 445480-73-9 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[[[2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

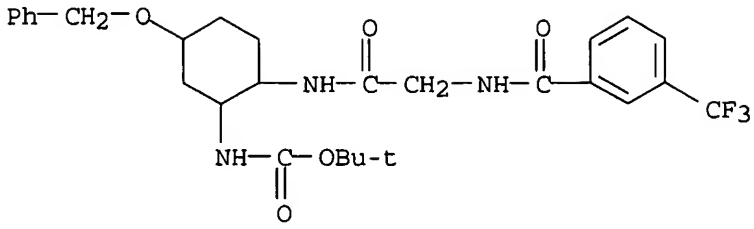
Relative stereochemistry.



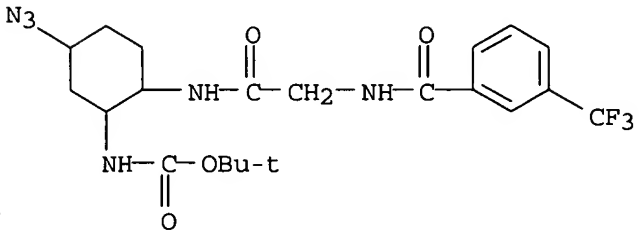
RN 445480-75-1 CAPLUS
CN Carbamic acid, [2-[[[[2-[(4-morpholinylcarbonyl)amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



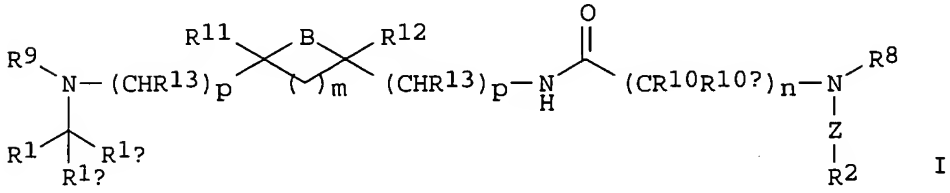
RN 445481-13-0 CAPLUS
CN Carbamic acid, [5-(phenylmethoxy)-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



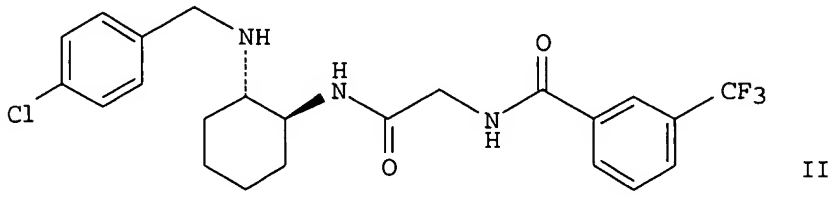
RN 445481-14-1 CAPLUS
CN Carbamic acid, [5-azido-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



GI



I



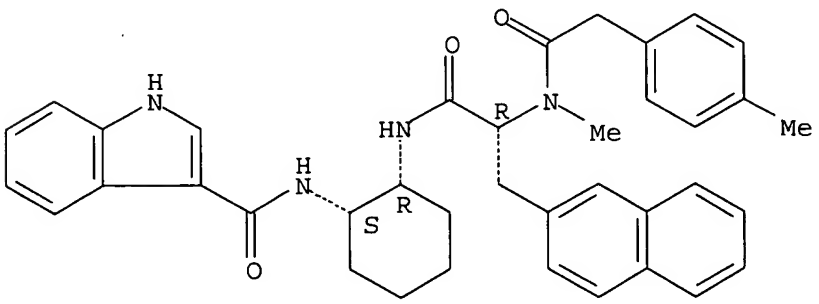
II

AB Title compds. I [wherein; or pharmaceutically acceptable salts thereof] were prepared as modulators of chemokine receptor activity, especially monocyte chemoattractant protein-1 (MCP-1) (no data). For example, N-tert-butoxycarbonylcyclohexane-(S,S)-1,2-diamine was treated with 4-methylmorpholine and [[3-(trifluoromethyl)benzoyl]amino]acetic acid in DMF to give the amide. Deprotection using TFA in CH2Cl2, followed by sequential addition of Hunig's base, 4-chlorobenzaldehyde, and NaHB(OAc)3, afforded the [(cyclohexylamino)oxoethyl]benzamide II. I are useful for the treatment and prevention of inflammatory disease, allergic and autoimmune diseases, and in particular, rheumatoid arthritis, multiple

sclerosis, atherosclerosis and asthma (no data).

L11 ANSWER 22 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:484021 CAPLUS
DOCUMENT NUMBER: 137:379900
TITLE: Pharmacology of MEN 11467: a potent new selective and orally-effective peptidomimetic tachykinin NK1 receptor antagonist
AUTHOR(S): Cirillo, R.; Astolfi, M.; Conte, B.; Lopez, G.; Parlani, M.; Sacco, G.; Terracciano, R.; Fincham, C. I.; Sisto, A.; Evangelista, S.; Maggi, C. A.; Manzini, S.
CORPORATE SOURCE: Department of Pharmacology, Menarini Ricerche SpA, Pomezia-Roma, I-00040, Italy
SOURCE: Neuropeptides (Edinburgh, United Kingdom) (2001), 35(3&4), 137-147
CODEN: NRPPDD; ISSN: 0143-4179
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **214487-46-4**, MEN 11467
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. of a potent new selective and orally-effective peptidomimetic tachykinin NK1 receptor antagonist, MEN 11467)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



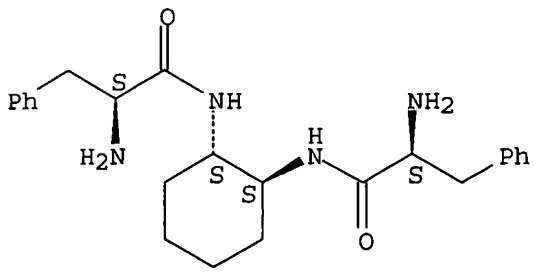
AB We have investigated the pharmacol. properties of MEN 11467, a novel partially retro-inverse peptidomimetic antagonist of tachykinin NK1 receptors. MEN 11467 potently inhibits the binding of [3H] substance P (SP) to tachykinin NK1 receptors in the IM9 limphoblastoid cell line (pKi = 9.4±0.1). MEN 11467 is highly specific for the human tachykinin NK1 receptors, since it has negligible effects (pKi <6) on the binding of specific ligands to tachykinin NK2 or NK3 receptors and to a panel of 30 receptors ion channels unrelated to tachykinin receptors. The antagonism exerted by MEN 11467 at tachykinin NK1 receptors is insurmountable in saturation binding expts., both KD and Bmax of SP were significantly reduced by MEN 11467 (0.3-10 nM). In the guinea-pig isolated ileum, MEN 11467 (0.03-1 nM) produced a nonparallel rightward shift of the concentration-response curve to SP methylester with a concomitant reduction of the Emax to the agonist (pKB = 10.7±0.1). Moreover the antagonist activity of MEN

11467 was hardly reversible despite prolonged washout. In vivo, MEN 11467 produced a long lasting (> 2-3 h) dose-dependent antagonism of bronchoconstriction induced by the selective tachykinin NK1 receptor agonist, [Sar9, Met(O2)11]SP in anesthetized guinea-pigs (ID50s' = 29±5, 31±12 and 670±270 μg/kg, after i.v., intranasal and intraduodenal administration, resp.), without affecting bronchoconstriction induced by methacholine. After oral administration MEN 11467 produced a dose-dependent inhibition of plasma protein extravasation induced in guinea-pig bronchi by [Sar9, Met(O2)11] (ID50 = 6.7±2 mg/kg) or by antigen challenge in sensitized animals (ID50 = 1.3 mg/kg). After i.v. administration MEN 11467 weakly inhibited the GR 73632-induced foot tapping behavior in gerbil (ED50 = 2.96±2 mg/kg), indicating a poor ability to block central tachykinin NK1 receptors. These results demonstrate that MEN 11467 is a potent, highly selective and orally effective insurmountable pseudopeptide antagonist of peripheral tachykinin NK1 receptors with a long duration of action.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

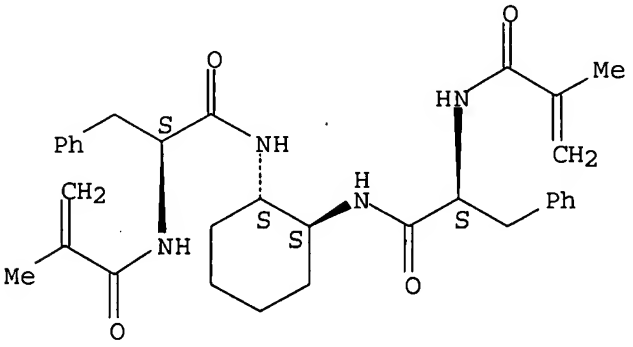
L11 ANSWER 23 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:311304 CAPLUS
DOCUMENT NUMBER: 137:149471
TITLE: New CSPs based on peptidomimetics: efficient chiral selectors in enantioselective separations
AUTHOR(S): Burguete, M. Isabel; Frechet, Jean M. J.; Garcia-Verdugo, Eduardo; Janco, Miroslav; Luis, Santiago V.; Svec, Frantisek; Vicent, Maria J.; Xu, Mingcheng
CORPORATE SOURCE: Department of Inorganic and Organic Chemistry, E.S.T.C.E. Universitat Jaume I, Castellon, E-12080, Spain
SOURCE: Polymer Bulletin (Berlin, Germany) (2002), 48(1), 9-15
CODEN: POBUDR; ISSN: 0170-0839
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **444891-04-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of chiral stationary phases based on peptidomimetics for enantioselective sepns.)
RN 444891-04-7 CAPLUS
CN Benzenepropanamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[α-amino-, (αS,α'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **444647-78-3P**
RL: ARU (Analytical role, unclassified); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent)
(peptidomimetics; preparation of chiral stationary phases based on peptidomimetics for enantioselective sepns.)
RN 444647-78-3 CAPLUS
CN Benzenepropanamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[α-[(2-methyl-1-oxo-2-propenyl)amino]-, (αS,α'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

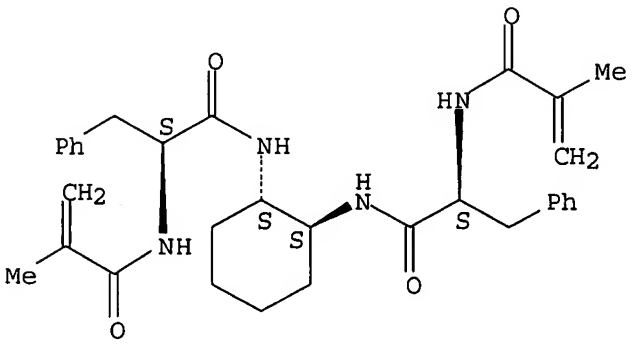


IT **444647-82-9P 444647-83-0P**
RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of chiral stationary phases based on peptidomimetics for enantioselective sepns.)
RN 444647-82-9 CAPLUS
CN Benzenepropanamide, N,N'-(1S,2S)-1,2-cyclohexanediylbis[α-[(2-methyl-1-oxo-2-propenyl)amino]-, (αS,α'S)-, polymer with diethenylbenzene and ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 444647-78-3
CMF C32 H40 N4 O4

Absolute stereochemistry.



CM 2

CRN 1321-74-0
CMF C10 H10
CCI IDS

2 [D1—CH═CH2]

CM 3

CRN 100-42-5
CMF C8 H8

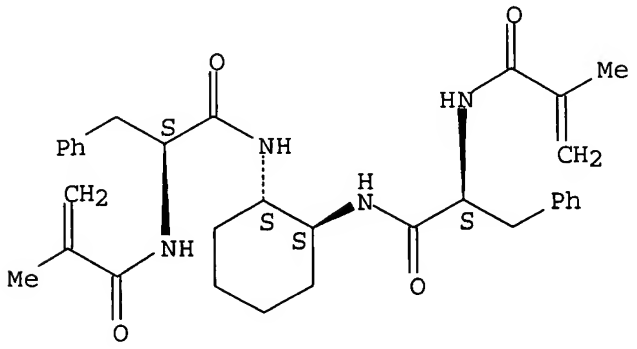
H2C═CH—Ph

RN 444647-83-0 CAPLUS
CN 2-Propenoic acid, 2-methyl-, 2-ethyl-2-[[(2-methyl-1-oxo-2-propenyl)oxy]methyl]-1,3-propanediyl ester, polymer with methyl 2-methyl-2-propenoate and (αS,α'S)-N,N'-(1S,2S)-1,2-cyclohexanediylbis[α-[(2-methyl-1-oxo-2-propenyl)amino]benzenepropanamide] (9CI) (CA INDEX NAME)

CM 1

CRN 444647-78-3
CMF C32 H40 N4 O4

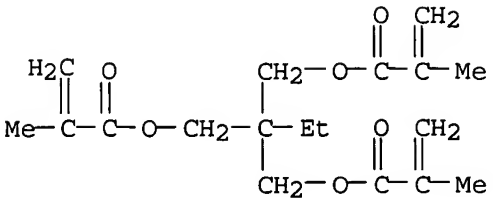
Absolute stereochemistry.



CM 2

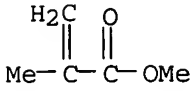
CRN 3290-92-4

CMF C18 H26 O6



CM 3

CRN 80-62-6
CMF C5 H8 O2



AB Two different families of peptidomimetics were synthesized and used as chiral selectors for enantioselective chromatog. The functionalization of compds. with multiple nitrogen atoms allows their use in the preparation of chiral stationary phases (CSPs), with acrylic or styril comonomers, in both bead and monolithic formats. Some of these separation media, having the appropriate morphol. properties for their use in chromatog. columns, were able to efficiently discriminate enantiomers of amino acid derivs. and pharmaceuticals such as oxazepam.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 24 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:923610 CAPLUS
DOCUMENT NUMBER: 136:31709
TITLE: Method of treating symptoms of hormonal variation, including hot flashes, using a tachykinin receptor antagonist
INVENTOR(S): Guttuso, Thomas J., Jr.
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095904	A1	20011220	WO 2001-US40924	20010612

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

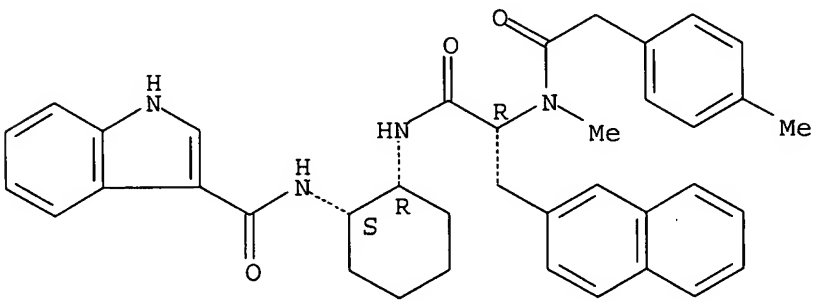
CA 2412355	AA	20011220	CA 2001-2412355	20010612
US 2002016283	A1	20020207	US 2001-879390	20010612
EP 1299100	A1	20030409	EP 2001-942248	20010612
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003236237	A1	20031225	US 2003-609176	20030627
PRIORITY APPLN. INFO.:			US 2000-211116P	P 20000612
			US 2001-879390	A1 20010612
			WO 2001-US40924	W 20010612

IT **214487-46-4**, MEN 11467
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tachykinin receptor antagonist for treating symptoms of hormonal variation, including hot flashes)

RN 214487-46-4 CAPLUS

CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Methods are provided for treating hot flashes and symptoms of hormonal variation in a patient, which methods include providing a tachykinin receptor antagonist and administering the tachykinin receptor antagonist to a patient experiencing a symptom of hormonal variation under conditions effective to treat the symptom of hormonal variation, which symptoms of hormonal variation can include hot flashes.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

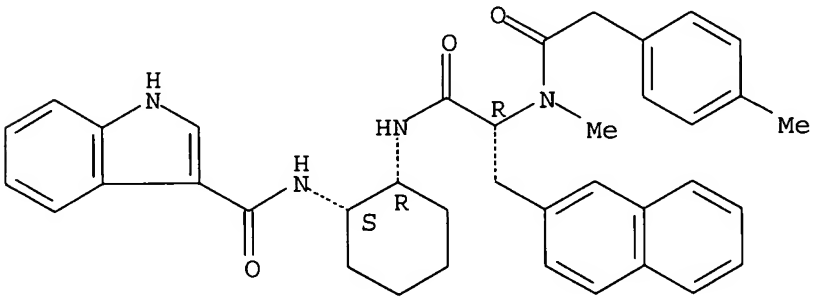
L11 ANSWER 25 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	2001:523530 CAPLUS
DOCUMENT NUMBER:	135:111983
TITLE:	NK1-Receptor antagonists for the treatment of the restless leg syndrome
INVENTOR(S):	Brecht, Hans-Michael; Jung, Birgit
PATENT ASSIGNEE(S):	Boehringer Ingelheim Pharma K.-G., Germany
SOURCE:	Ger. Offen., 4 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10001785	A1	20010719	DE 2000-10001785	20000118
WO 2001052854	A1	20010726	WO 2001-EP263	20010111
W: CA, JP, MX, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 2001034320	A1	20011025	US 2001-764629	20010118
PRIORITY APPLN. INFO.:			DE 2000-10001785 A	20000118
			US 2000-180399P P	20000204

IT **214487-46-4**, MEN 11467
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(NK1-receptor antagonists for treatment of restless leg syndrome)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

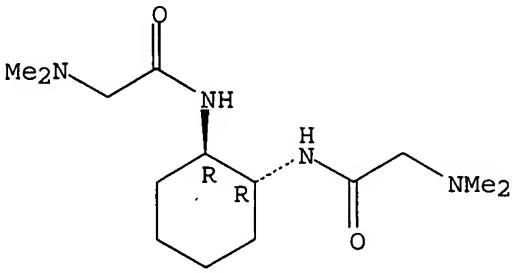


AB The invention concerns the use from NK1-receptor antagonists for the production of a drug for the treatment of the restless leg syndrome. The drugs are selected from e.g., Neuronorm, BIF 1149, FK 888, SR 48968, SR 140333, and LY 303870. Opioids, α2-adrenoceptor agonists, and Antiparkinsonian agents may be used in conjunction with NK1-receptor antagonists.

L11 ANSWER 26 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:457135 CAPLUS
DOCUMENT NUMBER: 135:256988
TITLE: A practical and efficient synthesis of chiral N,N-disubstituted C2 symmetric diamines derived from (R,R)-1,2-diaminocyclohexane
AUTHOR(S): Alexakis, A.; Chauvin, A.-S.; Stouvenel, R.; Vrancken, E.; Mutti, S.; Mangeney, P.
CORPORATE SOURCE: Department of Organic Chemistry, University of Geneva, Geneva, CH-1211, Switz.
SOURCE: Tetrahedron: Asymmetry (2001), 12(8), 1171-1178
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:256988
IT **361382-28-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(N-alkylation of diaminocyclohexane)

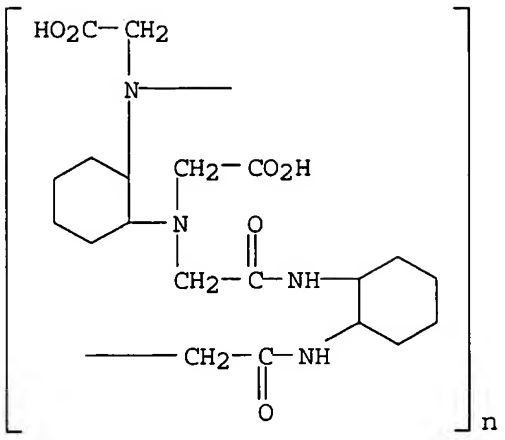
RN 361382-28-7 CAPLUS
CN Acetamide, N,N'-(1R,2R)-1,2-cyclohexanediylbis[2-(dimethylamino)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB An improved synthesis of chiral diamine ligands derived from (R,R)-1,2-diaminocyclohexane is described, providing N-substituted diamines. The synthesis of other new ligands based on this methodol. is also reported.
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

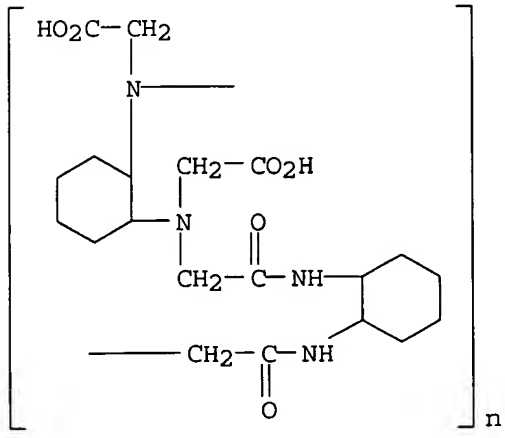
L11 ANSWER 27 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:271293 CAPLUS
DOCUMENT NUMBER: 134:367567
TITLE: Synthesis of soluble complexan polymers in organic solvents for using as a polymer-chelate precursor to YBa2Cu3O7-x thin films
AUTHOR(S): Naka, Kensuke; Tanaka, Yasuyuki; Yamasaki, Kunitoshi; Ohki, Akira; Chujo, Yoshiki; Maeda, Shigeru
CORPORATE SOURCE: Department of Polymer Chemistry, Graduate School of Engineering, Kyoto university, Kyoto, 606-8501, Japan
SOURCE: Bulletin of the Chemical Society of Japan (2001), 74(3), 571-577
CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **340320-89-0DP**, metal complexes
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of soluble complex polymers in organic solvents for using as a polymer-chelate precursor to YBa2Cu3O7-x thin films)
RN 340320-89-0 CAPLUS
CN Poly[[(carboxymethyl)imino]-(1R,2R)-1,2-cyclohexanediyl[(carboxymethyl)imino](2-oxo-1,2-ethanediyl)imino-(1R,2R)-1,2-cyclohexanediylimino(1-oxo-1,2-ethanediyl)], rel- (9CI) (CA INDEX NAME)



IT **340320-89-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of soluble complex polymers in organic solvents for using as a polymer-chelate precursor to YBa2Cu3O7-x thin films)

RN 340320-89-0 CAPLUS

CN Poly[[(carboxymethyl)imino]-(1R,2R)-1,2-cyclohexanediyl[(carboxymethyl)imino](2-oxo-1,2-ethanediyl)imino-(1R,2R)-1,2-cyclohexanediylimino(1-oxo-1,2-ethanediyl)], rel- (9CI) (CA INDEX NAME)



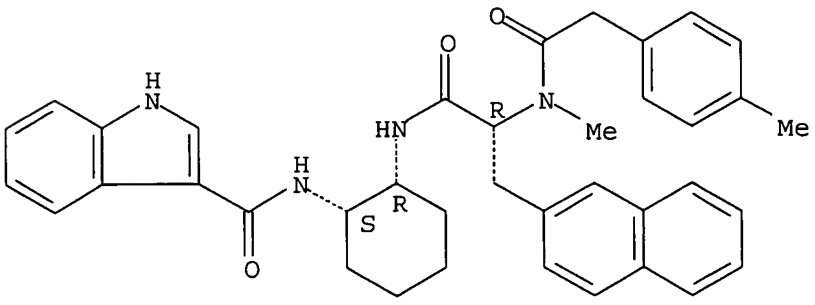
AB A soluble complexan polymer in organic solvents, derived from 1,2-diaminocyclohexane-N,N,N',N'-tetraacetic acid (CyDTA), was synthesized and used as a polymer chelate precursor to YBa2Cu3O7-x thin films. Five complexan polymers (3) were prepared by a ring-opening polyaddn. of CyDTA dianhydride (1) with several diamines (2). The polymer (3e) prepared with 1,2-diaminocyclohexane (2e) was soluble in water, DMSO (DMSO), methanol, and ethanol. A clear aqueous solution (pH 8) containing 3e and 1/2 equiv molar amount of metal nitrates of Y, Ba, and Cu (1:2:3 in molar ratio) was poured into tetrahydrofurane (THF) to precipitate a polymer-metal chelate. The chelate formations of each metal were confirmed by C=O stretching bonds. The polymer chelate precursor was soluble in methanol, DMSO, and water, and partially soluble in ethanol. The polymer-metal chelate was dissolved in

methanol, of which the metal concentration was adjusted to 3 wt%. This solution was spin-coated onto SrTiO3 (100) and MgO (001) substrates for preparing YBa2Cu3O7-x thin films. According to an X-ray diffraction anal., YBa2Cu3O7-x film with a c-axis orientation was formed on a SrTiO3 substrate; even the precursor film was sintered at 780 °C for 1 h under air. Superconducting YBa2Cu3O7-x films with a c-axis orientation were also prepared on a MgO (001) substrate.

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 28 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:114146 CAPLUS
DOCUMENT NUMBER: 134:290215
TITLE: Effect of the long-acting tachykinin NK1 receptor antagonist MEN 11467 on tracheal mucus secretion in allergic ferrets
AUTHOR(S): Khan, Safina; Liu, Yu-Chih; Khawaja, Aamir M.; Manzini, Stefano; Rogers, Duncan F.
CORPORATE SOURCE: Thoracic Medicine, National Heart & Lung Institute, Imperial College, London, SW3 6LY, UK
SOURCE: British Journal of Pharmacology (2001), 132(1), 189-196
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **214487-46-4**, MEN 11467
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of tachykinin NK1 receptor antagonist MEN 11467 on tracheal mucus secretion in allergic ferrets)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB We investigated the effect of MEN 11467 ((1R,2S)-2-N[1(H)indol-3-yl-carbonyl]-1-N-{Nα(p-tolylacetyl)-Nα(methyl)-D-3-(2-naphthyl)alanyl}diaminocyclohexane) on tachykinin-induced mucus secretion in ferret trachea in vitro and determined its effect on secretion by tracheae from allergic ferrets in response to allergen challenge. Repeated administration of [Sar9,Met(O2)11]-substance P ([Sar9]SP, 1 μM) maintained mucus output above control values for at least 1.75 h. MEN

11467 inhibited secretion in a concentration-dependent manner with maximal inhibition at 10 μM and an approx. IC50 of 0.3 μM. Inhibition by MEN 11467 (0.1-10 μM) was maintained, to varying degree, for at least 1.75 h after washout in the continued presence of [Sar9]SP. In elec. stimulated tracheae, tachykininergic neural secretion was virtually abolished by 1 μM MEN 11467. In tracheae from ovalbumin-sensitized animals, repeated administration of ovalbumin maintained mucus output above controls for 1.5 h. MEN 11467 inhibited ovalbumin-induced secretion in a concentration-dependent manner, with complete inhibition at 1 μM. Inhibition by MEN 11467 (1 and 10 μM) was maintained, to varying degree, after drug washout for the 1.5 h of ovalbumin stimulation. MEN 11467 1 μM did not affect secretion induced by either acetylcholine or histamine, whereas 10 μM MEN 11467 did inhibit agonist-induced secretion. We conclude that, in ferret trachea in vitro, MEN 11467 at concns. of 0.1-1 μM is a long acting and selective inhibitor of tachykininergic-induced mucus secretion, and may have therapeutic potential for bronchial hypersecretion associated with allergic conditions, for example in asthma.

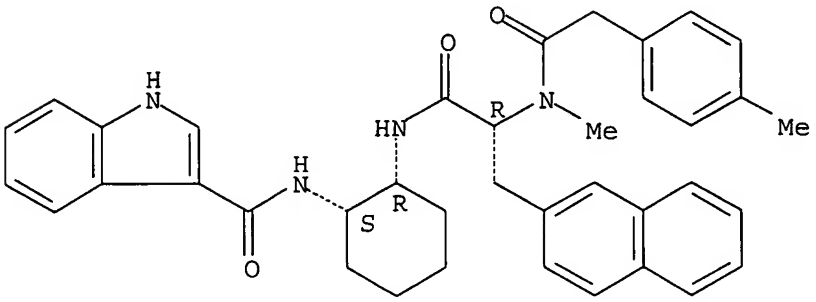
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 29 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:31282 CAPLUS
DOCUMENT NUMBER: 134:80813
TITLE: Use of substance P antagonists in the treatment of adenocarcinomas
INVENTOR(S): Pompei, Pierluigi; Massi, Maurizio; Nabissi, Massimo; Sparapani, Pier Luigi
PATENT ASSIGNEE(S): Innova Limited, UK
SOURCE: PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001001922	A2	20010111	WO 2000-EP6309	20000705
WO 2001001922	A3	20010510		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
IT 1306165	B1	20010530	IT 1999-RM426	19990705
CA 2373960	AA	20010111	CA 2000-2373960	20000705
AU 2000065616	A5	20010122	AU 2000-65616	20000705
EP 1206259	A2	20020522	EP 2000-953011	20000705
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003503429	T2	20030128	JP 2001-507420	20000705
US 6576638	B1	20030610	US 2002-30305	20020513
PRIORITY APPLN. INFO.:			IT 1999-RM426 A	19990705
			WO 2000-EP6309 W	20000705

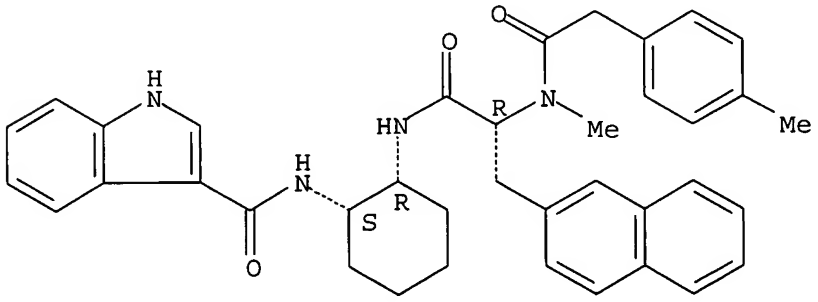
IT **214487-46-4**, MEN 11467 **214487-46-4D**, MEN 11467, derivs.
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(substance P antagonists in treatment of adenocarcinoma)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

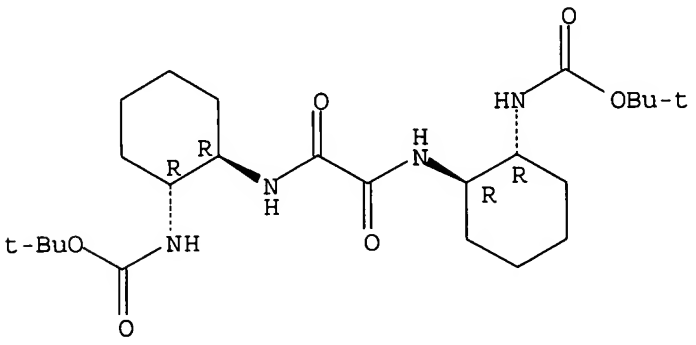


AB The invention discloses the use of antagonists of neurokinin receptors (NK-1; substance P receptors) to establish a new drug effective in the treatment of adenocarcinomas, the antagonists being ≥1 substances selected among those ones having the following features: pA2>6.0 both in human and in murine tissues, etherocyclic non-peptidergic structures, antiangiogenic effects exptl. demonstrated in genitourinary tract tumors induced via orthotopic grafts of human tumor cells either in the genitourinary apparatus of either immunodeficient rats or mice, decrease of tumor mass on tumors of the genitourinary tract induced by orthotopic grafts of tumor cells onto tissues of the genitourinary tract of either immunodeficient rats or mice.

L11 ANSWER 30 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:836249 CAPLUS
DOCUMENT NUMBER: 134:147352
TITLE: Amide catalysts with tetradentate ligands and the

asymmetric transfer hydrogenation of carbonyl compounds
AUTHOR(S): Marson, C. M.; Schwarz, I.
CORPORATE SOURCE: Department of Chemistry, University College London, Christopher Ingold Laboratories, London, WC1H OAJ, UK
SOURCE: Tetrahedron Letters (2000), 41(46), 8999-9003
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:147352
IT **323187-43-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amidic tetradentate ligands as catalysts for asym. transfer hydrogenation of carbonyl compds.)
RN 323187-43-5 CAPLUS
CN Carbamic acid, [(1,2-dioxo-1,2-ethanediyl)bis[imino-(1R,2R)-2,1-cyclohexanediyl]]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Amidic tetradentate catalysts comprising two trans-1,2-cyclohexanediamine units linked via a dicarbonyl spacer are shown to provide useful enantiomeric excesses in the asym. transfer hydrogenation from propan-2-ol to aromatic ketones. N-benzylation of the terminal amino groups results, in several cases, in reversal of the absolute configuration of the major product.
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 31 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:628111 CAPLUS
DOCUMENT NUMBER: 133:222443
TITLE: Regioselective synthesis of DTPA derivatives
INVENTOR(S): Chinn, Paul; Gyorkos, Albert; Labarre, Michael J.; Ruhl, Steve; Ryskamp, Thomas
PATENT ASSIGNEE(S): Idec Pharmaceuticals Corporation, USA
SOURCE: PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2000051976	A1	20000908	WO 2000-US5433	20000302
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6207858	B1	20010327	US 1999-261207	19990303
CA 2364960	AA	20000908	CA 2000-2364960	20000302
EP 1157004	A1	20011128	EP 2000-913703	20000302
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008693	A	20011226	BR 2000-8693	20000302
AU 778816	B2	20041223	AU 2000-35099	20000302
ZA 2001006750	A	20021115	ZA 2001-6750	20010815
NO 2001004194	A	20011026	NO 2001-4194	20010829
PRIORITY APPLN. INFO.:			US 1999-261207 A	19990303
			WO 2000-US5433 W	20000302

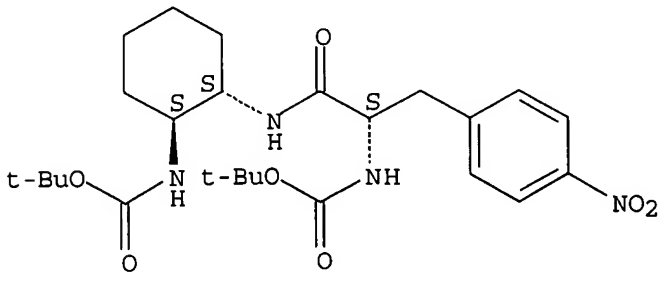
OTHER SOURCE(S): CASREACT 133:222443

IT **290836-17-8P**
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(regioselective synthesis of DTPA derivs.)

RN 290836-17-8 CAPLUS

CN Carbamic acid, [(1S)-2-[[(1S,2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]cyclohexyl]amino]-1-[(4-nitrophenyl)methyl]-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



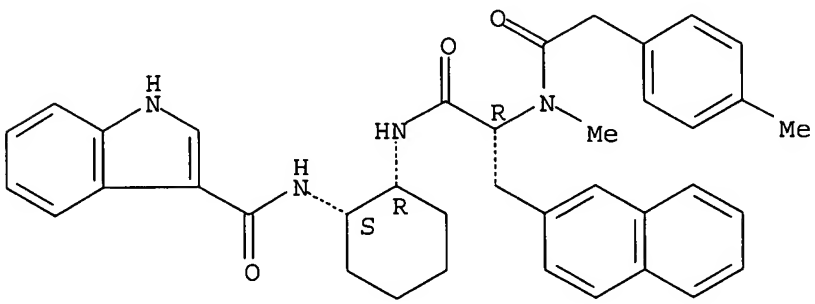
AB The title process for synthesizing a substantially isomerically pure DTPA derivative (sic) comprises regioselective coupling a monoprotected diamine and, e.g., a compound comprising an amine moiety capable of effectively coupling the DTPA derivative to Igs (sic). Thus, 4-(O2N)C6H4CH2CH(NHCO2CMe3)CO2H was coupled with H2NCHMeCH2NHCO2CMe3 to give 71.83% 4-(O2N)C6H4CH2CH(NHCO2CMe3)CONHCH2CHMeCH2NHCO2CMe3 which was converted in 5 addnl. steps to MX-DTPA.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 32 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:92927 CAPLUS
DOCUMENT NUMBER: 133:362

TITLE: Anti-tumor activity of tachykinin NK1 receptor antagonists on human glioma U373 MG xenograft
AUTHOR(S): Palma, C.; Bigioni, M.; Irrissuto, C.; Nardelli, F.; Maggi, C. A.; Manzini, S.
CORPORATE SOURCE: Menarini Ricerche S.p.A., Department of Pharmacology, Pomezia, 00040, Italy
SOURCE: British Journal of Cancer (2000), 82(2), 480-487
CODEN: BJCAAI; ISSN: 0007-0920
PUBLISHER: Churchill Livingstone
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **214487-46-4**, MEN 11467
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tachykinin NK1 receptor antagonists antitumor activity on human glioma)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

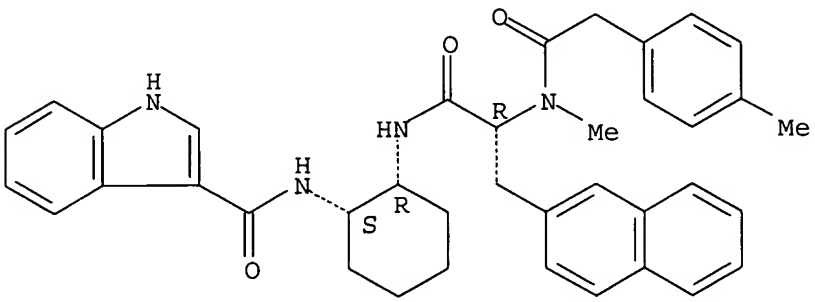


AB Astrocytes harbor functional receptors to many neurotransmitters, including substance P (SP), an undecapeptide belonging to the tachykinin family of peptide transmitters. SP activates malignant glial cells to induce cytokine release and proliferation, both responses being relevant for tumor progression. In tumors developed in nude mice transplanted s.c. (s.c.) to U373 MG human glioma cells, the presence of SP was observed at immunohistochem. Although the administration of exogenous SP did not significantly affect the size or development of U373 MG xenograft, a role of SP in supporting glioma progression in vivo was highlighted by the tumor growth inhibition induced by highly specific and selective human tachykinin NK1 receptor antagonists (MEN 11467 and MEN 11149). The anti-tumor activity of MEN 11467 was observed both with s.c. or i.v. treatments and was partially reverted by the concomitant administration of exogenous SP. Doxorubicin did not show any activity in controlling U373 MG growth in this in vivo model. A novel therapeutic approach to treat malignant gliomas with tachykinin NK1 receptor antagonists is suggested by these findings.
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 33 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:466663 CAPLUS
DOCUMENT NUMBER: 131:194198

TITLE: Correlation between binding characteristics and functional antagonism in human glioma cells by tachykinin NK1 receptor antagonists
AUTHOR(S): Palma, Carla; Nardelli, Federica; Manzini, Stefano
CORPORATE SOURCE: Department of Pharmacology, Menarini Ricerche, Rome, 00040, Italy
SOURCE: European Journal of Pharmacology (1999), 374(3), 435-443
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **214487-46-4**, MEN 11467
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(binding characteristics and functional antagonism in human glioma cells by tachykinin NK1 receptor antagonists)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



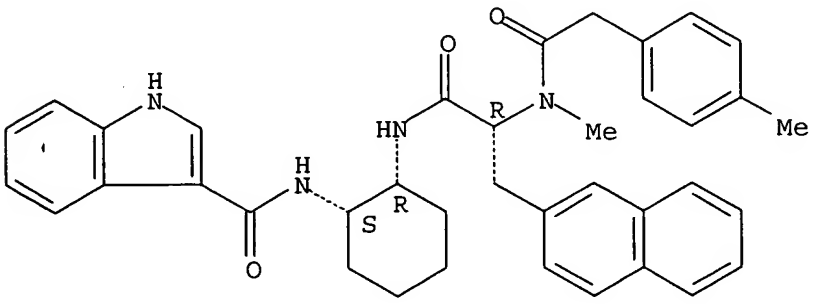
AB Binding characteristics and functional antagonism exerted by two structurally related tachykinin NK1 receptor antagonists, MEN 11467 ((1R,2S)-2N[1(H)indol-3-yl-carbonyl]-1-N-{Nα(p-tolylacetyl)-Nα(methyl)-D-3-(2-naphthyl)alanyl}diaminocyclohexane) and FK888 (N2-[(4R)-4-hydroxy-1-(1-methyl-1H-indol-3-yl)carbonyl-L-prolyl]-N-methyl-N-phenylmethyl-L-3-(2-naphthyl)alaninamide), were investigated in the human astrocytoma cell line U373 MG. In radioligand binding studies, conducted with [3H]substance P and intact cells at 37°C, MEN 11467 bound to tachykinin NK1 receptors in an irreversible manner with a Ki value of 1.2 ± 0.5 nM while FK888 bound in competitive manner with a Ki value of 4.6 ± 2.2 nM. Receptor blockade by both antagonists resulted in a powerful and complete inhibition of functional responses induced by substance P, such as accumulation of the second messenger inositol monophosphate or interleukin-6 release. However, MEN 11467 showed a greater potency for blocking functional responses than FK888 despite their similar affinity for human tachykinin NK1 receptors. Moreover, MEN 11467 was more potent in inhibiting late rather than early phases of substance P-induced inositol monophosphate accumulation and its antagonism was enhanced by drug preincubation and barely affected by removal of unbound drug from the external medium, suggesting that MEN 11467 bound in a tight manner to the receptor. Such behavior was not observed with the competitive and rapidly reversible antagonist FK888. These data indicate that the small differences in the chemical structure of MEN 11467 and FK888 determine the

different binding characteristics at the tachykinin NK1 receptor and which are responsible for the greater potency of MEN 11467 for blocking functional responses. The Ki value obtained in binding studies may be inadequate to reveal the real potency of tachykinin NK1 receptor antagonists.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 34 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:449800 CAPLUS
DOCUMENT NUMBER: 131:252257
TITLE: Effect of MEN 11467, a new tachykinin NK1 receptor antagonist, in acute rectocolitis induced by acetic acid in guinea-pigs
AUTHOR(S): Cutrufo, Corrado; Evangelista, Stefano; Cirillo, Rocco; Ciucci, Alessandra; Conte, Bruno; Lopez, Giuseppe; Manzini, Stefano; Maggi, Carlo Alberto
CORPORATE SOURCE: Department of Pharmacology, Menarini Ricerche spa, Rome, Italy
SOURCE: European Journal of Pharmacology (1999), 374(2), 277-283
CODEN: EJPHAZ; ISSN: 0014-2999
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **214487-46-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect of MEN 11467, a new tachykinin NK1 receptor antagonist, in acute rectocolitis induced by acetic acid in guinea-pigs)
RN 214487-46-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[(1S,2R)-2-[[(2R)-2-[methyl[(4-methylphenyl)acetyl]amino]-3-(2-naphthalenyl)-1-oxopropyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The aim of this study was to evaluate the effect of MEN 11467, a new potent tachykinin NK1 receptor antagonist, in an exptl. model of acute rectocolitis induced by an enema with 7.5% acetic acid in guinea-pigs. This effect was compared to that of mesalazine (5-amino-2-hydroxybenzoic acid). The injury was quantified visually by using a macroscopic injury score and histol. by using a necrosis score. In addition, changes in myeloperoxidase activity, a marker for neutrophil infiltration, and plasma protein extravasation were evaluated. The injury caused by 7.5% acetic acid was mild, affecting the superficial layers and producing a strong

edema of the submucosa. A single administration of MEN 11467 (0.3-10 mg/kg s.c., 1 h before acetic acid) reduced the macroscopic damage and necrosis score and the increase in plasma protein extravasation induced by 7.5% acetic acid in the early acute phase of the injury (death at 2.5 h). Mesalazine (100 mg/kg p.o., 1 h before) reduced the macroscopic score but not the plasma protein extravasation. Repeated administration of MEN 11467 (1-3 mg/kg s.c., -1, +6 and +23 h after 7.5% acetic acid) reduced the macroscopic score and myeloperoxidase activity but not the plasma protein extravasation induced in the late phase of acute injury (death at 24 h). At this time mesalazine markedly reduced the macroscopic score, myeloperoxidase activity and plasma protein extravasation induced by 7.5% acetic acid. These results suggest a greater involvement of tachykinin NK1 receptors in the early phase than in the late phase of colonic inflammation in response to chemical injury.

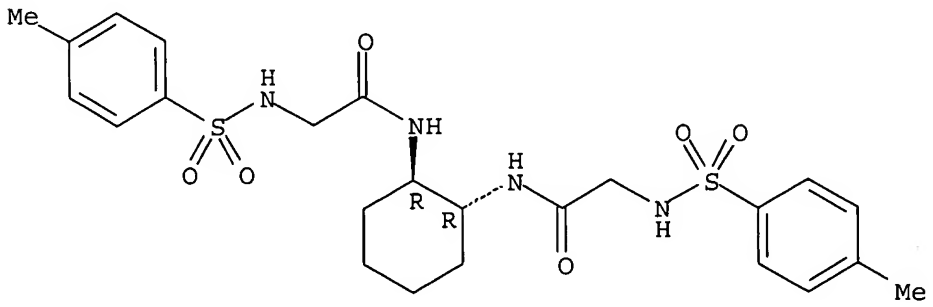
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 37 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:436043 CAPLUS
DOCUMENT NUMBER: 127:105963
TITLE: Toward the Rational Design of Superoxide Dismutase Mimics: Mechanistic Studies for the Elucidation of Substituent Effects on the Catalytic Activity of Macrocyclic Manganese(II) Complexes
AUTHOR(S): Riley, Dennis P.; Lennon, Patrick J.; Neumann, William L.; Weiss, Randy H.
CORPORATE SOURCE: Monsanto Company, St. Louis, MO, 63167, USA
SOURCE: Journal of the American Chemical Society (1997), 119(28), 6522-6528
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **192319-86-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(superoxide dismutase mimics - catalytic activity of macrocyclic manganese(II) complexes)

RN 192319-86-1 CAPLUS
CN Acetamide, N,N'-1,2-cyclohexanediylbis[2-[[(4-methylphenyl)sulfonyl]amino]-, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Two new isomeric bis(trans-fused cyclohexano) substituted

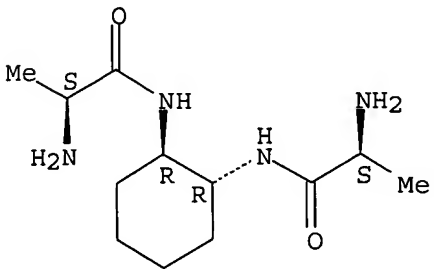
1,4,7,10,13-pentaazacyclopentadecane ligands and their Mn(II) complexes, (I) and (II), have been synthesized, and their activity as superoxide dismutase (SOD) catalysts has studied. Complex I is an excellent SOD catalyst with a second-order rate constant at pH = 7.4 of 1.2+108 M-1 s-1. In contrast, the isomeric complex II has virtually no detectable catalytic SOD activity, implying the need to understand the effect that the position, number, and stereochem. of substituents exert on the catalytic rate. The crystal structure of the complex II was determined and reveals that the Mn(II) ion is coordinated in a pentagonal bipyramid array of the five nitrogens of the macrocyclic ligand and capped by two trans-chloro ligands. Crystal data for MnC18H37Cl2N5 are as follows: triclinic at 20°, space group P1--Ci2 (number 2); a = 9.746(3) Å, b = 12.631(6) Å, c = 11.311(5) Å; α = 73.14(4)°, β = 76.39(3)°, γ = 79.98(3)°, V = 1287(1) Å3, and Z = 2 (ρcalc = 1.279 g/cm3; μa Mo Kα = 6.23 mm-1). Mechanistic studies with the complex I and the pentamethyl substituted complex, including D2O rate studies, are reported and are consistent with the existence of two pathways for the rate-determining electron-transfer from Mn(II) to superoxide: (1) hydrogen atom transfer from a bound water on Mn(II) to HO2• to yield a Mn(III) hydro intermediate and (2) the dissociative pathway in which superoxide anion binds to a vacant coordination site on Mn(II) followed by protonation/oxidation to yield a Mn(III)hydroperoxo species. Subsequent reduction of the intermediate Mn(III) with superoxide anion completes the catalytic cycle. Substituent effects on the rates and relative contribution of the two pathways to the overall rate of SOD activity is ascribed to the propensity of the ligand to fold around Mn(II) forming a pseudo-octahedral complex similar in geometry to the oxidized Mn(III) complex. Folding of the pentaaza macrocyclic ligand is confirmed as a relevant structural motif for this series of Mn(II) complexes by the x-ray structure determination of the bis(nitrate) derivative, [Mn(C10H25N5)NO3]NO3, which reveals a six-coordinate structure with a folded conformation of the macrocyclic ligand. Crystal data for [Mn(C10H25N5)NO3]NO3: orthorhombic at -100°C, space group P212121; a = 9.457(2) Å, b = 12.758(2) Å, c = 13.834(2) Å, V = 1669.1(5) Å3, and Z = 4 (ρcalc = 1.549 g/cm3).

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 38 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:612907 CAPLUS
DOCUMENT NUMBER: 125:315168
TITLE: Cobalt(III) complexes of N,N'-bis(2(S)-aminopropyl)-1(R),2(R)-trans-1,2-diaminocyclohexane
AUTHOR(S): Lee, Dong-Il; Jun, Moo-Jin
CORPORATE SOURCE: Dep. of Chemistry, Yonsei Univ., Seoul, 120-749, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1996), 17(9), 786-790
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **183255-16-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of optically active bis(aminopropyl)diaminocyclohexane and its cobalt complexes)

RN 183255-16-5 CAPLUS
CN Propanamide, N,N'-1,2-cyclohexanediylbis[2-amino-, dihydrochloride, [1R-[1α(S*),2β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



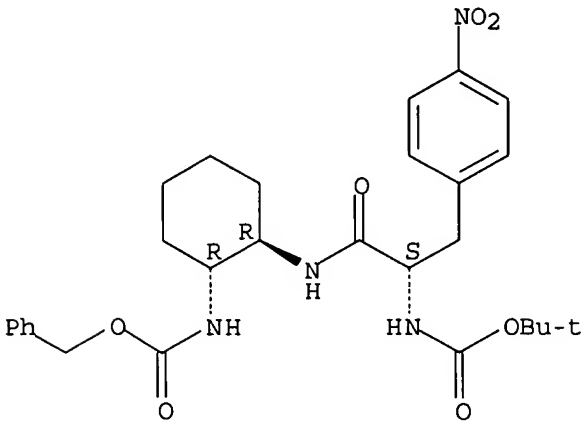
● 2 HCl

AB A novel optically active tetraamine ligand possessing four asym. centers, N,N'-bis(2(S)-aminopropyl)-1(R),2(R)-trans-1,2-diaminocyclohexane (SRRS-apchxn) and its cobalt(III) complexes, [Co(SRRS-apchxn)X2]n+ (X = Cl-, H2O; X2 = CO32-) were synthesized. This ligand has coordinated stereospecifically to the cobalt(III) ion to give only the Λ-uns-cis(SS) isomer. A trans dichloro complex was obtained via the stereospecific isomerization of Λ-uns-cis(SS)-[Co(SRRS-apchxn)Cl2]+ to trans-(SS)-[Co(SRRS-apchxn)Cl2]+ in CH3OH-HCl medium. Ligand and complexes were characterized by electronic absorption, 1H NMR, CD spectra, and also by elemental anal. It is of interest that this is one of the few CoIII(N4)X2 type complex prepns., which produces such an uns-cis isomer with stereospecificity.

L11 ANSWER 41 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:448054 CAPLUS
DOCUMENT NUMBER: 117:48054
TITLE: Synthesis of C-functionalized trans-cyclohexyldiethylenetriaminepentaacetic acids for labeling of monoclonal antibodies with the bismuth-212 α-particle emitter
AUTHOR(S): Brechbiel, Martin W.; Gansow, Otto A.
CORPORATE SOURCE: Radiat. Oncol. Branch, Natl. Cancer Inst., Bethesda, MD, 20892, USA
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (9), 1173-8
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:48054
IT **142350-86-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrogen bromide)
RN 142350-86-5 CAPLUS
CN Carbamic acid, [2-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(4-

nitrophenyl)-1-oxopropyl]amino]cyclohexyl]-, phenylmethyl ester, [1R-[1α,2β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Several C-functionalized cyclohexyldiethylenetriaminepentaacetic acid derivs. have been prepared from (±)-4-nitrophenylalanine and (±)-trans-cyclohexane-1,2-diamine to produce two sets of diastereoisomeric enantiomers. A modification of this synthesis has been employed to prepare a single enantiomer in order to define the absolute configurations of the products.

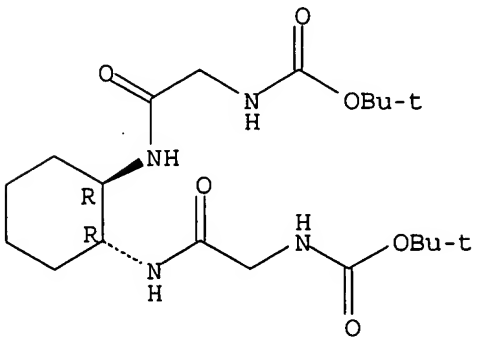
L11 ANSWER 42 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:443667 CAPLUS
DOCUMENT NUMBER: 117:43667
TITLE: N,N'-(2-aminoethyl)-trans-1,2-diaminocyclohexane-N,N',N'',N'',N''',N'''-hexaacetic acid and related compounds for chelating agents for immunoconjugates
INVENTOR(S): Mease, Ronnie C.; Srivastava, Suresh C.; Gestin, Jean Francois
PATENT ASSIGNEE(S): Associated Universities, Inc., USA
SOURCE: U.S., 13 pp. Cont.-in-part of U.S. 5,021,571.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5089663	A	19920218	US 1991-679258	19910402
US 5021571	A	19910604	US 1989-372905	19890629
US 5334729	A	19940802	US 1991-787244	19911104
PRIORITY APPLN. INFO.:			US 1989-372905 A2	19890629
			US 1991-679258 A3	19910402

IT **137731-40-9P 137731-42-1P 137820-29-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in cyclohexyl polyaminocarboxylate derivative preparation for radiolabeled immunoconjugate preparation)
RN 137731-40-9 CAPLUS
CN Carbamic acid, [1,2-cyclohexanediylbis[imino(2-oxo-2,1-ethanediyl)]]bis-,

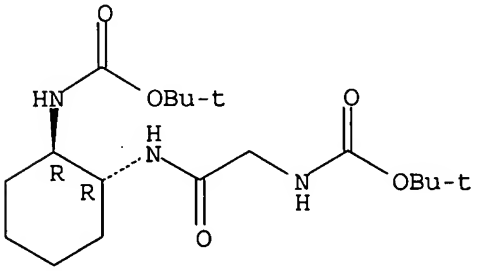
bis(1,1-dimethylethyl) ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



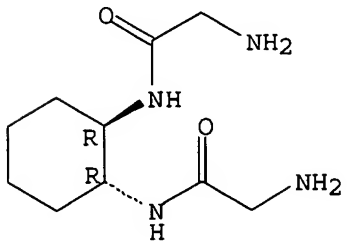
RN 137731-42-1 CAPLUS
CN Carbamic acid, [2-[[[[(1,1-dimethylethoxy)carbonyl]amino]acetyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 137820-29-2 CAPLUS
CN Acetamide, N,N'-1,2-cyclohexanediylbis[2-amino-, dihydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

AB Rigid chelating structures are disclosed, as are their preparation and their use in preparing radiometal-labeled immunoconjugates. The compds. of the

invention include cyclohexyl EDTA monoanhydride, the trans forms of cyclohexyl DTPA and TTHA, and derivs. of these cyclohexyl polyaminocarboxylate materials. The title compound is specifically claimed. Biodistribution of radiometal-labeled immunoconjugates is included. Cyclohexyl EDTA immunoconjugates (from both monoanhydride and N-hydroxysuccinimide derivs.) with anti-colon cancer antibody 17-1A were superior to the nonrigid counterparts with respect to tumor uptake.

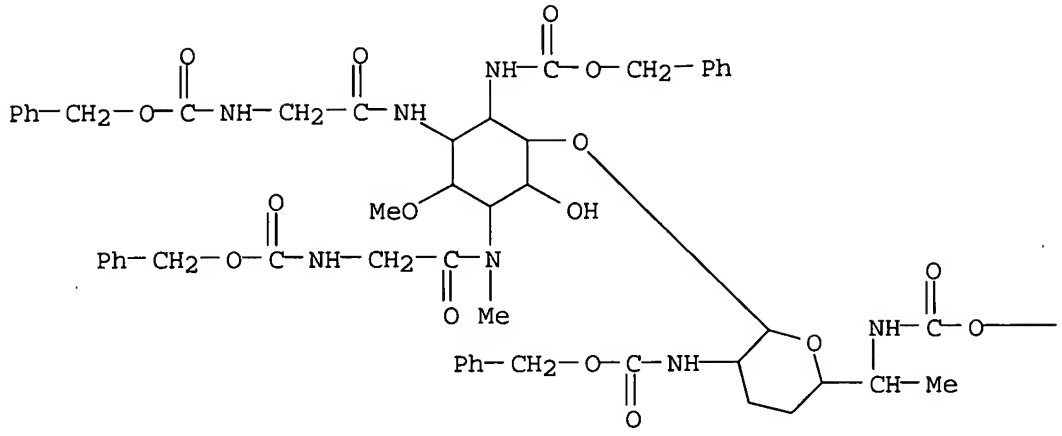
L11 ANSWER 46 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:498228 CAPLUS
DOCUMENT NUMBER: 95:98228
TITLE: 2-Deoxy-2-substituted fortimicin A and B and derivatives
INVENTOR(S): Johnson, Paulette; Martin, Jerry R.; Nadzan, Alex M.; Tadanier, John S.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S., 13 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4250304	A	19810210	US 1979-79145	19790926
AU 8061991	A1	19810402	AU 1980-61991	19800903
GB 2059958	A	19810429	GB 1980-29336	19800911
ES 495313	A1	19811016	ES 1980-495313	19800924
BE 885402	A1	19810325	BE 1980-202235	19800925
FR 2465743	A1	19810327	FR 1980-20601	19800925
FR 2465743	B1	19830708		
DE 3036185	A1	19810416	DE 1980-3036185	19800925
JP 56057799	A2	19810520	JP 1980-133150	19800926

PRIORITY APPLN. INFO.: US 1979-79145 A 19790926

IT **78027-31-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 78027-31-3 CAPLUS
CN L-chiro-Inositol, 1,4,5-trideoxy-6-O-methyl-1-[methyl[[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-3-O-[2,3,4,6,7-pentadeoxy-2,6-bis[[(phenylmethoxy)carbonyl]amino]-β-L-lyxo-heptopyranosyl]-4-[[(phenylmethoxy)carbonyl]amino]-5-[[[[(phenylmethoxy)carbonyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

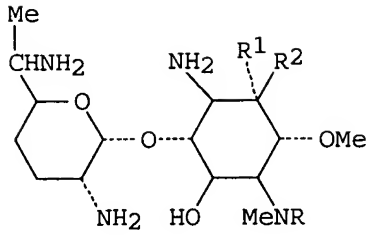
PAGE 1-A



PAGE 1-B

—CH_2—Ph

GI



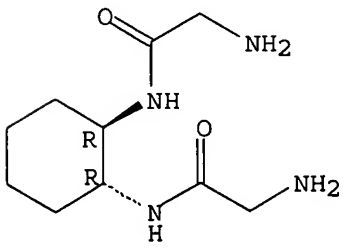
I

AB Fortimicins I (R = H, glycyl, β-alanyl, Ac, β-aminoalkyl; R1 = H, NH2, N3, halo, glycylamido, β-alanylamido, 2-O-methanesulfonyl; R2 = H, halo; R1 = R2 ≠ H), with antibacterial activity, were prepared Thus, fortimicin B in 4 steps was converted into 1,2',6'-tri-N-benzyloxycarbonyl-2-O-methanesulfonylfortimicin B, which was treated with N-hydroxysuccinimide ester of N-benzyloxycarbonylglycine and the product hydrogenolyzed over Pd/C to give 2-O-methanesulfonylfortimicin A.4HCl

(II). A solution of II was passed through a column of anion exchange resin, basic eluate was allowed to stand at room temperature for 120 h, the solution was concentrated and again was passed through an anion exchange resin column to give 2-deoxy-1,2-epiminofortimicin A, which was treated with NaN3 to give I.4HCl (R = H2NCH2CO, R1 = N3, R2 = H) (III). Min. inhibitory concentration of III against Staphylococcus aureus Smith is 3.1 μg/mL.

L11 ANSWER 47 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1974:485380 CAPLUS
DOCUMENT NUMBER: 81:85380
TITLE: Stereochemical studies of N-methyl-(S)-alaninatocobalt(III) complexes with chiral tetramines. II. Cobalt(III)-N-methyl-(S)- and (R)-alaninate-N,N'-bis(β-aminoethyl)-1(R), 2(R)-diaminocyclohexane systems
AUTHOR(S): Saburi, Masahiko; Yoshikawa, Sadao
CORPORATE SOURCE: Fac. Eng., Univ. Tokyo, Tokyo, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1974), 47(5), 1184-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **53719-90-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53719-90-7 CAPLUS
CN Acetamide, N,N'-1,2-cyclohexanediylbis[2-amino-, dihydrochloride, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

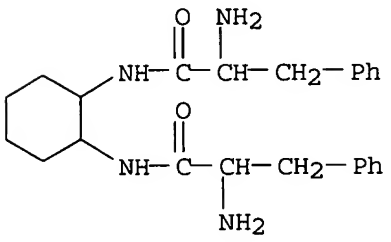


●2 HCl

GI For diagram(s), see printed CA Issue.
AB The preparation and structural assignments of N-methyl-(S)- and -(R)-alaninato-cobalt(III) complexes with N,N'-bis(β-aminoethyl)-1(R),-2(R)-diaminocyclohexane[(R)-baetchxn] are described. The Λ-β2(SSR) isomer I was obtained for Co(N-Me-(S)-Ala)[(R)-baetchxn]2+ ion. The two isomers, which were found for the Co-[N-Me-(R)-Ala] [(R)-baetchnx]2+ ion under equilibrium condition at pH 7, are assigned as the Λ-β2(SSR) and Λ-β2(SSS) configurations, taking into account the stereospecific coordination of the (R)-baetchxn. The stereoisomerism of Δ-β2-Co(N-Me-(S)-Ala)(trien)2+ ion is also discussed. The structures of 2 species observed in the

PMR measurements of Co(N-Me-(R)-Ala) ((R)-baet-chxn)2+ ion and assigned to Λ-β2(SSR) II and Λ-β2(SSS) III configurations, resp., are determined, based on the chemical shifts of α-methine protons of N-methylalaninate moieties.

L11 ANSWER 49 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:501371 CAPLUS
DOCUMENT NUMBER: 71:101371
TITLE: Synthesis of a new triethylenetetramine homolog containing four optically pure centers. Some stereoselective cobalt(III) ion complexes of this ligand
AUTHOR(S): Asperger, Robert G.
CORPORATE SOURCE: Biochem. Res. Lab., Dow Chem. Co., Midland, MI, USA
SOURCE: Inorganic Chemistry (1969), 8(10), 2127-31
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **24125-68-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 24125-68-6 CAPLUS
CN Hydrocinnamamide, N,N'-1,2-cyclohexylenebis[α-amino-, dihydrochloride (8CI) (CA INDEX NAME)



●2 HCl

GI For diagram(s), see printed CA Issue.
AB The synthesis of a new tetramine ligand, N,N'-bis(L-2-amino-3-phenylpropyl)-trans-D-1,2-cyclohexanediamine (I), a homolog of triethylene-tetramine which contains four optical centers, is reported. The syntheses of the L-cis-β- and optically active trans-cobalt(III) perchlorate derivs. are reported. Absorption and O.R.D. spectra are reported and used, along with some chemical data, to assign the configurations of the isomer.

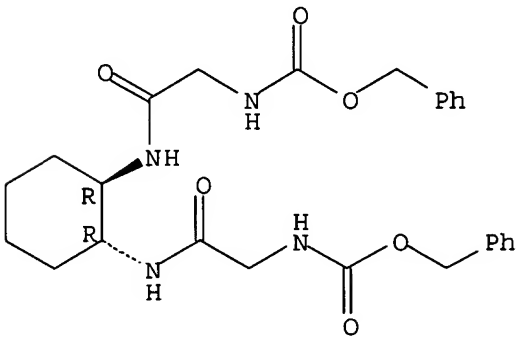
L11 ANSWER 50 OF 50 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:73647 CAPLUS
DOCUMENT NUMBER: 70:73647
TITLE: Stereochemical studies of metal chelates. III. Preparation and stereochemistry of cobalt(III) complexes with C-substituted triethylenetetramines at the central ethylenediamine bridge
AUTHOR(S): Goto, Masafumi; Saburi, Masahiko; Yoshikawa, Sadao
CORPORATE SOURCE: Univ. Tokyo, Tokyo, Japan

SOURCE: Inorganic Chemistry (1969), 8(2), 358-66
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **22559-12-2P 22559-13-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

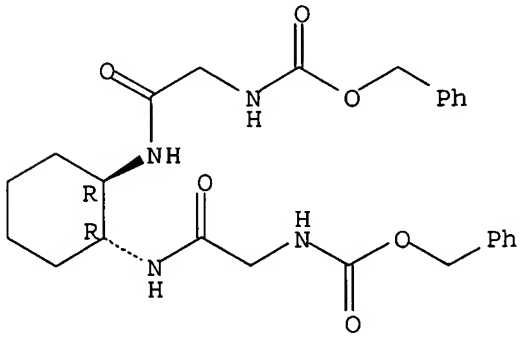
RN 22559-12-2 CAPLUS
CN Carbamic acid, [1,2-cyclohexylenebis(iminocarbonylmethylene)]di-, dibenzyl ester, trans- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 22559-13-3 CAPLUS
CN Carbamic acid, [1,2-cyclohexanediylbis[imino(2-oxo-2,1-ethanediyl)]]bis-, bis(phenylmethyl) ester, (1R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB The preparation of dichloro- and dinitrocobalt(III) complexes of optically active C-substituted triethylenetetramine at the central ethylenediamine bridge is described. The stereoselective formation of the cis-β isomer was observed and the stereochem. details are discussed in terms of the conformation of each chelate ring as well as the configurations of the secondary N atoms. The rearrangement of cis-β-dichloro complexes to trans-isomers is also reported.

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